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Chapter 1

Landau-Fermi-liquid theory: Phenomenology

One of the first thing that one learns in a Solid State Physics course is that the thermodynamic and transport properties of metals are well described in terms of non-interacting electrons; the Drude-Sommerfeld-Boltzmann theory of metals. Yet, this evidence is somehow surprising in view of the fact that actual electrons interact mutually via Coulomb repulsion, which is not weak at all.

This puzzle was solved brilliantly in the end of the 50's by Landau, as we are going to discuss in what follows. We will start by analysing the case of a neutral Fermi system, like ${}^3\text{He}$. Later we shall discuss charged Fermi systems, relevant to metals.

1.1 The Landau energy functional and the concept of quasiparticles

Let us start from a non-interacting Fermi gas at very low temperature T . Right at $T = 0$ we know that the ground state is the Fermi sea that is obtained by filling with two opposite-spin electrons all momentum states with energy smaller than the chemical potential μ (the Fermi energy). In other words, if $n_{\mathbf{k}\sigma}$ is the occupation number of each momentum state – $n_{\mathbf{k}\sigma}$ being zero or one because of Pauli principle – then the Fermi-sea occupation numbers are

$$n_{\mathbf{k}\sigma}^{(0)} = \begin{cases} 1 & \text{if } \epsilon_{\mathbf{k}}^{(0)} \leq \mu \\ 0 & \text{if } \epsilon_{\mathbf{k}}^{(0)} > \mu \end{cases}.$$

At finite temperature, the equilibrium values of the occupation numbers are given by the Fermi-Dirac distribution

$$n_{\mathbf{k}\sigma}^{(0)} = f(\epsilon_{\mathbf{k}}^{(0)} - \mu) = (1 + e^{\beta(\epsilon_{\mathbf{k}}^{(0)} - \mu)})^{-1},$$

with $\beta = 1/K_B T$ the inverse temperature. Any excited state can be uniquely identified by the variation of the occupation numbers with respect to equilibrium, namely through

$$\delta n_{\mathbf{k}\sigma} = n_{\mathbf{k}\sigma} - n_{\mathbf{k}\sigma}^{(0)}, \quad (1.1)$$

and costs an energy

$$\delta E^{(0)} [\{\delta n_{\mathbf{p}\alpha}\}] = \sum_{\mathbf{k}\sigma} (\epsilon_{\mathbf{k}}^{(0)} - \mu) \delta n_{\mathbf{k}\sigma}, \quad (1.2)$$

that is a simple functional of the $\delta n_{\mathbf{k}\sigma}$'s.

Now suppose that we switch on smoothly the interaction. Each non-interacting excited state will evolve smoothly into a fully-interacting one. The Landau hypothesis was that the non-interacting and the fully interacting states are *adiabatically connected*; in other words they are in one-to-one correspondence. This implies in particular that each fully-interacting excited state can be uniquely identified, like its non-interacting partner, by the deviation with respect to equilibrium of the occupation numbers $\delta n_{\mathbf{k}\sigma}$. Consequently, its excitation energy δE must be a functional of the $\delta n_{\mathbf{k}\sigma}$'s, i.e.

$$\delta E [\{\delta n_{\mathbf{p}\alpha}\}]. \quad (1.3)$$

Remark

This hypothesis may look simple but it is actually deeply counter-intuitive. Suppose we have a “non-interacting” Hamiltonian \mathcal{H}_0 and a fully-interacting one $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$, and suppose to follow the spectrum, that we assume discrete, within a specific symmetry-subspace of the Hamiltonian

$$\mathcal{H}(\lambda) = \mathcal{H}_0 + \lambda \mathcal{H}_1,$$

with λ that increases smoothly from 0 to 1. The evolution of the spectrum must resemble that one drawn schematically in Fig. 1.1 with a series of avoided crossings that allow to follow adiabatically the n -th excited level at $\lambda = 0$ into the n -th excited level at $\lambda = 1$. Note that the crossing are avoided because the states have the same symmetry. If we were to consider levels of different symmetries nothing would prevent crossings. However, while the adiabatic evolution does occur and it is a well accepted phenomenon in models with discrete spectra, it is equally common wisdom that it can not happen when the spectrum is continuous, as in a bulk metal. Landau’s revolutionary hypothesis that the adiabatic evolution also occurs in a bulk system, at least for the low energy excited states, and the fact that, by this simple assumption, one can justify and predict a lot of physical properties is one of the major achievements of the contemporary Condensed Matter Theory.

Let us therefore assume that the excitation energy of the fully-interacting Fermi system is indeed a functional of the same $\delta n_{\mathbf{k}\sigma}$'s as its non-interacting partner, and further suppose

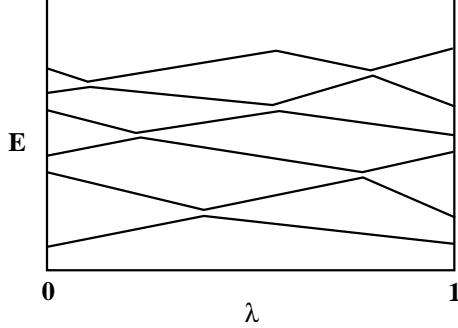


Figure 1.1: Adiabatic evolution of a discrete spectrum within a specific symmetry-subspace.

that the temperature is very small. In this case, any weak deviation from equilibrium must correspond to $\delta n_{\mathbf{k}\sigma} \ll 1$, that justifies a Taylor expansion of (1.3), namely

$$\delta E [\{\delta n_{\mathbf{p}\alpha}\}] = \sum_{\mathbf{k}\sigma} (\epsilon_{\mathbf{k}\sigma} - \mu) \delta n_{\mathbf{k}\sigma} + \frac{1}{2} \sum_{\mathbf{k}\mathbf{k}'} \sum_{\sigma\sigma'} f_{\mathbf{k}\sigma \mathbf{k}'\sigma'} \delta n_{\mathbf{k}\sigma} \delta n_{\mathbf{k}'\sigma'} + O(\delta n^3). \quad (1.4)$$

This is the famous Landau's energy functional. Note that

- even though the two terms are apparently of different orders, in reality they are of the same order since the excitation energies $\epsilon_{\mathbf{k}\sigma} - \mu$ are of the same order as the deviations of the occupation numbers;
- $\epsilon_{\mathbf{k}\sigma}$ should not be confused with the non-interacting energies $\epsilon_{\mathbf{k}\sigma}^{(0)}$.

Rigorously speaking, the $\delta n_{\mathbf{k}\sigma}$'s that appear in (1.4) only serve as labels to identify excited states and they do not correspond to deviations of the occupation numbers of the real particles, as in the non-interacting case (1.2). Just for this reason, Landau coined for $\delta n_{\mathbf{k}\sigma}$ the definition “quasiparticle” occupation number, as if the real-particle excitations were substituted in the presence of interaction by “quasiparticle” excitations. The Fermi gas of these quasiparticles is the so-called “Landau-Fermi liquid”.

Remark

This idea is actually ubiquitous in all Solid State Physics. Let us for instance recall briefly how phonons arise. One starts from a model of interacting ions and electrons. Because of their larger mass with respect to the electrons and of the Coulomb interaction among them and with the electrons, the ions localize, thus forming a lattice, and the low energy excitations become the small fluctuations around the equilibrium positions, whose quantization gives rise to phonons, which are bosons. In other words, one begins with real particles, the ions, yet their low-energy

excitations in the presence of interaction are new bosonic “quasiparticles”, the phonons, that turns out to be generally weakly interacting among each other and with the electrons. This allows to treat such an interaction within perturbation theory, unlike the original Coulomb interaction. In a more general context, since the only many-body systems that can be solved exactly in any dimensions are free bosons or fermions, it is a very natural, and fortunately successful, approach to attempt a description of the low-energy excitations of, even strongly, interacting models in terms of effective “quasiparticles”, bosons or fermions, whose interaction is weak enough to be treated perturbatively.

Going back to the Landau energy functional (1.4), in the case in which spin isotropy is preserved the following equivalences hold:

$$f_{\mathbf{k}\uparrow\mathbf{k}'\uparrow} = f_{\mathbf{k}\downarrow\mathbf{k}'\downarrow}, \quad f_{\mathbf{k}\uparrow\mathbf{k}'\downarrow} = f_{\mathbf{k}\downarrow\mathbf{k}'\uparrow}.$$

In this case, the choice of a spin quantization axis must not be influential, hence it is convenient to rewrite (1.4) in a form that is explicitly spin isotropic. For that purpose, let us introduce charge deviations from equilibrium

$$\delta\rho_{\mathbf{k}} = \delta n_{\mathbf{k}\uparrow} + \delta n_{\mathbf{k}\downarrow}, \quad (1.5)$$

and spin ones

$$\delta\sigma_{\mathbf{k}} = (\delta\sigma_{\mathbf{k}}^x, \delta\sigma_{\mathbf{k}}^y, \delta\sigma_{\mathbf{k}}^z), \quad (1.6)$$

where the z -component is simply

$$\delta\sigma_{\mathbf{k}}^z = \delta n_{\mathbf{k}\uparrow} - \delta n_{\mathbf{k}\downarrow}.$$

With these definitions the second term of the energy functional (1.4) can be written as

$$\frac{1}{2} \sum_{\mathbf{k}\mathbf{k}'} f_{\mathbf{k}\mathbf{k}'}^S \delta\rho_{\mathbf{k}} \delta\rho_{\mathbf{k}'} + f_{\mathbf{k}\mathbf{k}'}^A \delta\sigma_{\mathbf{k}} \cdot \delta\sigma_{\mathbf{k}'}, \quad (1.7)$$

where

$$f^S = \frac{1}{2} (f_{\uparrow\uparrow} + f_{\uparrow\downarrow}), \quad f^A = \frac{1}{2} (f_{\uparrow\uparrow} - f_{\uparrow\downarrow}), \quad (1.8)$$

as can be readily demonstrated by equating (1.4) and (1.7) assuming a deviation from equilibrium of the form

$$\delta\sigma_{\mathbf{k}} = (0, 0, \delta\sigma_{\mathbf{k}}^z).$$

1.2 Quasiparticle thermodynamics

Let us derive, starting from the Landau's energy functional, the thermodynamical properties of the quasiparticles. We note that, if we consider a deviation from equilibrium that consists, in the absence of interaction, to add δN particles in particular momentum-states, i.e. an excited state identified by $\delta n_{\mathbf{k}\sigma}$ such that

$$\sum_{\mathbf{k}\sigma} \delta n_{\mathbf{k}\sigma} = \delta N, \quad (1.9)$$

such a state must evolve in the Landau's hypothesis into a state with the same “quasiparticle” excitations $\delta n_{\mathbf{k}\sigma}$ and furthermore, since the total number of particles is conserved along the adiabatic evolution, with the same deviation δN from equilibrium. In other words, although quasiparticles have not to be confused with real particles, still the sum of all quasiparticle deviations of the occupation numbers gives the variation of the total number of real particles, i.e. Eq. (1.9).

Remark

It is important to note that the adiabatic evolution hypothesis guarantees that only true conserved quantities, like the total number of particles or the total spin, keep the same expressions in terms of quasiparticle occupation numbers as for the real particles. Conserved quantities refer, rigorously speaking, only to the fully interacting Hamiltonian, whereas the non-interacting one has generally much larger symmetry. In other words, the Landau's theory of Fermi liquid has only to do with conserved quantities but its use is not at all justified for non-conserved ones, even if they are conserved in the non-interacting limit. This fact is often underestimated and may lead easily to wrong conclusions.

Since the labelling of the states is identical to non-interacting electrons, the phase-space volume counting is the same, hence also the formal expression of the entropy-change δS :

$$\delta S = \delta \left[-K_B \sum_{\mathbf{k}\sigma} n_{\mathbf{k}\sigma} \ln n_{\mathbf{k}\sigma} + (1 - n_{\mathbf{k}\sigma}) \ln (1 - n_{\mathbf{k}\sigma}) \right]. \quad (1.10)$$

Thermodynamic equilibrium implies an extremum of the free-energy F , namely that

$$\delta F = \delta E - T \delta S - \mu \delta N = 0. \quad (1.11)$$

Let us solve this equation by assuming that the deviation from equilibrium is induced by a deviation of the quasiparticle occupation numbers $\delta n_{\mathbf{k}\sigma}$, that amounts to impose

$$\left(\frac{\delta F}{\delta n_{\mathbf{k}\sigma}} \right)_{\delta n=0} = 0.$$

By Eq. (1.4) we find that

$$\frac{\delta E}{\delta n_{\mathbf{k}\sigma}} = \epsilon_{\mathbf{k}} + \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma\mathbf{k}'\sigma'} \delta n_{\mathbf{k}'\sigma'} \equiv \bar{\epsilon}_{\mathbf{k}\sigma}, \quad (1.12)$$

is the quasiparticle energy in the presence of excited quasiparticles, including itself, while what it is needed is

$$\left(\frac{\delta E}{\delta n_{\mathbf{k}\sigma}} \right)_{\delta n=0} = \epsilon_{\mathbf{k}},$$

that is obviously independent of δn . Since all terms in (1.11) have exactly the same expression as for non-interacting particles, one readily realizes that the quasiparticle equilibrium distribution is the Fermi-Dirac distribution

$$n_{\mathbf{k}\sigma}^0 = n_{\mathbf{k}}^0 = f(\epsilon_{\mathbf{k}} - \mu) = \left(1 + e^{\beta(\epsilon_{\mathbf{k}} - \mu)} \right)^{-1}, \quad (1.13)$$

the only difference with respect to non-interacting real particles being the renormalized band dispersion $\epsilon_{\mathbf{k}}$.

We must point out that $f(\epsilon_{\mathbf{k}} - \mu)$ corresponds to global equilibrium – all quasiparticles are in equilibrium among themselves. Analogously, we could define a distribution function for the “local” equilibrium that minimizes the free-energy of a single excited quasiparticle in the presence of other excited quasiparticles. It is clear from Eq. (1.12) that the local-equilibrium distribution function is the Fermi-Dirac distribution with argument the quasiparticle energy $\bar{\epsilon}_{\mathbf{k}\sigma}$, i.e.

$$\bar{n}_{\mathbf{k}\sigma}^0 = f(\bar{\epsilon}_{\mathbf{k}\sigma} - \mu) = \left(1 + e^{\beta(\bar{\epsilon}_{\mathbf{k}\sigma} - \mu)} \right)^{-1},$$

which is a functional of the occupation number deviations.

In accordance, we can define a deviation with respect to local equilibrium as

$$\delta \bar{n}_{\mathbf{k}\sigma} = n_{\mathbf{k}\sigma} - f(\bar{\epsilon}_{\mathbf{k}\sigma} - \mu), \quad (1.14)$$

as opposed to that one with respect to global equilibrium

$$\begin{aligned} \delta n_{\mathbf{k}\sigma} &= n_{\mathbf{k}\sigma} - n_{\mathbf{k}}^0 \\ &= \delta \bar{n}_{\mathbf{k}\sigma} + \bar{n}_{\mathbf{k}\sigma}^0 - n_{\mathbf{k}}^0 \\ &= \delta \bar{n}_{\mathbf{k}\sigma} + \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} (\bar{\epsilon}_{\mathbf{k}\sigma} - \epsilon_{\mathbf{k}\sigma}) \\ &= \delta \bar{n}_{\mathbf{k}\sigma} + \frac{\partial f(\epsilon_{\mathbf{k}} - \mu)}{\partial \epsilon_{\mathbf{k}}} (\bar{\epsilon}_{\mathbf{k}\sigma} - \epsilon_{\mathbf{k}\sigma}) \\ &\simeq \delta \bar{n}_{\mathbf{k}\sigma} - \delta(\epsilon_{\mathbf{k}} - \mu) \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma\mathbf{k}'\sigma'} \delta n_{\mathbf{k}'\sigma'}, \end{aligned} \quad (1.15)$$

where we have assumed to be close to equilibrium and at very low temperature.

Now let us consider, as conventionally done, a space-isotropic system, where $\epsilon_{\mathbf{k}} = \epsilon(|\mathbf{k}|)$ and use the parametrization

$$\delta n_{\mathbf{k}\sigma} = -\frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \sum_{lm} Y_{lm}(\Omega_{\mathbf{k}}) \delta n_{lm\sigma} \simeq \delta(\epsilon_{\mathbf{k}} - \mu) \sum_{lm} Y_{lm}(\Omega_{\mathbf{k}}) \delta n_{lm\sigma}, \quad (1.16)$$

where $Y_{lm}(\Omega_{\mathbf{k}})$ are spherical harmonics identified by the Euler angles of the unit vector in the direction of \mathbf{k} , being its modulus fixed by the δ -function to be right on the Fermi sphere. (The δ -function in the right hand side of (1.16) derives from the fact that both sides of that equation must consistently be of first order in the deviation from equilibrium.)

In addition, we introduce the Legendre decomposition of $f_{\mathbf{kk}'}$ assuming that it depends only on the relative angle $\theta_{\mathbf{kk}'}$ between the two momenta, their modula being on the Fermi sphere. Therefore

$$f_{\mathbf{kk}'}^{S(A)} = \sum_l f_l^{S(A)} P_l(\theta_{\mathbf{kk}'}), \quad (1.17)$$

where $P_l(\theta_{\mathbf{kk}'})$ are Legendre polynomials.¹ In the non-abelian representation in which the energy functional is explicitly spin-isotropic, one readily finds through (1.15) the following relations between the charge/spin deviations at global and local equilibrium:

$$\delta\rho_{\mathbf{k}} = \delta\bar{\rho}_{\mathbf{k}} + 2 \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \sum_{\mathbf{k}'} f_{\mathbf{kk}'}^S \delta\rho_{\mathbf{k}'}, \quad (1.18)$$

$$\delta\sigma_{\mathbf{k}} = \delta\bar{\sigma}_{\mathbf{k}} + 2 \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \sum_{\mathbf{k}'} f_{\mathbf{kk}'}^A \delta\sigma_{\mathbf{k}'}. \quad (1.19)$$

One realizes that, because of $\epsilon_{\mathbf{k}} = \epsilon(|\mathbf{k}|)$ and of the identity

$$\int \frac{d\Omega_{\mathbf{k}'}}{4\pi} P_l(\theta_{\mathbf{kk}'}) Y_{l'm'}(\Omega_{\mathbf{k}'}) = \delta_{ll'} \frac{1}{2l'+1} Y_{l'm'}(\Omega_{\mathbf{k}}),$$

it follows that

$$\begin{aligned} & - \sum_{\mathbf{k}'} \sum_l f_l^S P_l(\theta_{\mathbf{kk}'}) \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} Y_{l'm'}(\Omega_{\mathbf{k}'}) \delta\rho_{l'm'} \\ & \simeq \sum_{\mathbf{k}'} \sum_l f_l^S P_l(\theta_{\mathbf{kk}'}) \delta(\epsilon_{\mathbf{k}'} - \mu) \sum_{l'm'} Y_{l'm'}(\Omega_{\mathbf{k}'}) \delta\rho_{l'm'} \end{aligned}$$

¹Conventionally, the argument of the Legendre polynomials is indicated as $\cos\theta \in [-1 : 1]$. Here, in order to simplify notations, we have decided to use as argument θ

$$\begin{aligned}
&= \frac{V}{2} \mathcal{N} \sum_{ll'm'} f_l^S \delta\rho_{l'm'} \int \frac{d\Omega_{\mathbf{k}'}}{4\pi} P_l(\theta_{\mathbf{k}\mathbf{k}'}) Y_{l'm'}(\Omega_{\mathbf{k}'}) \\
&= \frac{V}{2} \mathcal{N} \sum_{l'm'} f_l^S \delta\rho_{l'm'} \frac{1}{2l'+1} Y_{l'm'}(\Omega_{\mathbf{k}}),
\end{aligned}$$

and analogously for $\delta\sigma_{\mathbf{k}}$ with $f^S \rightarrow f^A$, where $\mathcal{N} = \mathcal{N}(\mu)$ is the quasiparticle density of states

$$\mathcal{N}(\epsilon) = \frac{1}{V} \sum_{\mathbf{k}\sigma} \delta(\epsilon_{\mathbf{k}} - \epsilon),$$

at the chemical potential. Therefore Eqs. (1.18) and (1.19) have the simple solution

$$\delta\rho_{lm} = \frac{\delta\bar{\rho}_{lm}}{1 + \frac{F_l^S}{2l+1}}, \quad (1.20)$$

$$\delta\sigma_{lm} = \frac{\delta\bar{\sigma}_{lm}}{1 + \frac{F_l^A}{2l+1}}, \quad (1.21)$$

where the Landau F -parameters are defined through

$$F_l^{S(A)} = V \mathcal{N} f_l^{S(A)}. \quad (1.22)$$

It is also common to define A -parameters through

$$A_l^{S(A)} = \frac{F_l^{S(A)}}{1 + \frac{F_l^A}{2l+1}}, \quad (1.23)$$

so that

$$F_l^S \delta\rho_{lm} = A_l^S \delta\bar{\rho}_{lm}, \quad (1.24)$$

$$F_l^A \delta\sigma_{lm} = A_l^A \delta\bar{\sigma}_{lm}, \quad (1.25)$$

We note that the above formulas are valid only for an isotropic system, like ${}^3\text{He}$, or for a metal with an approximately spherical Fermi surface. In general, one must use, instead of spherical harmonics and Legendre polynomials, other basis functions appropriate to the symmetry of the lattice. However, in what follows we just take into account the isotropic case, unless otherwise stated.

1.2.1 Specific heat

Let us start the calculation of the quasiparticle thermodynamic properties at low temperature from the simplest one: the specific heat. It is easy to show through (1.10) (we set $K_B = 1$ as well as $\hbar = 1$) that

$$\begin{aligned} c_V &= \frac{T}{V} \left(\frac{\partial S}{\partial T} \right)_{N,V} \simeq \frac{T}{V} \left(\frac{\partial S}{\partial T} \right)_{\mu,V} + O(T^2) \\ &= -\frac{T}{V} \sum_{\mathbf{k}\sigma} \frac{\partial n_{\mathbf{k}}^0}{\partial T} \ln \frac{n_{\mathbf{k}\sigma}^0}{1 - n_{\mathbf{k}\sigma}^0} = -\frac{1}{TV} \sum_{\mathbf{k}\sigma} (\epsilon_{\mathbf{k}} - \mu)^2 \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \\ &= -\frac{1}{T} \int d\epsilon \mathcal{N}(\epsilon + \mu) \epsilon^2 \frac{\partial f(\epsilon)}{\partial \epsilon} = \frac{\pi^2}{3} \mathcal{N} T. \end{aligned} \quad (1.26)$$

This is the same expression as in the absence of interaction with the quasiparticle density of states \mathcal{N} instead of the free-particle one $\mathcal{N}^{(0)}$

$$\mathcal{N}^{(0)} = \mathcal{N}^{(0)}(\mu) = \sum_{\mathbf{k}\sigma} \delta \left(\epsilon_{\mathbf{k}}^{(0)} - \mu \right).$$

Therefore, if $c_V^{(0)}$ is the specific heat of the free particles, then

$$\frac{c_V}{c_V^{(0)}} = \frac{\mathcal{N}}{\mathcal{N}^{(0)}}. \quad (1.27)$$

1.2.2 Compressibility and magnetic susceptibility

Suppose that we perturb the system with a static homogeneous field that may modify the chemical potentials, $\mu_{\sigma} = \mu \rightarrow \mu + \delta\mu_{\sigma}$, for spin up and spin down real particles. At equilibrium, the quasiparticle occupation numbers will change accordingly as

$$\delta n_{\mathbf{k}\sigma} = \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} (\delta \epsilon_{\mathbf{k}\sigma} - \delta \mu_{\sigma}), \quad (1.28)$$

where

$$\delta \epsilon_{\mathbf{k}\sigma} = \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma \mathbf{k}'\sigma'} \delta n_{\mathbf{k}'\sigma'},$$

is the change in the quasiparticle energy due to the fact that the external field changes all quasiparticle occupation numbers. It is important to note that $\delta\mu_{\sigma}$ that appears in (1.28) coincides with the field that acts on the real particles because the latter couples to conserved quantities, otherwise nothing could guarantee that the two are equal. Once again this demonstrates that this theory only addresses the response of conserved quantities.

By means of Eq. (1.15) we find that

$$\delta\bar{n}_{\mathbf{k}\sigma} = \delta n_{\mathbf{k}\sigma} - \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma\mathbf{k}'\sigma'} \delta n_{\mathbf{k}'\sigma'} = -\frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \delta\mu_{\sigma}, \quad (1.29)$$

showing that the deviation from local equilibrium is the same as for free particles with dispersion $\epsilon_{\mathbf{k}}$ in the presence of the field.

Compressibility

The compressibility κ is defined by

$$\kappa = -\frac{1}{V} \frac{\partial V}{\partial P} = \frac{1}{n^2} \frac{\partial n}{\partial \mu},$$

where n is the total density. Since a variation in the total density of particles coincides with the variation in the quasiparticle one, we find through (1.20) that ²

$$\begin{aligned} \delta n &= \frac{1}{V} \sum_{\mathbf{k}\sigma} \delta n_{\mathbf{k}\sigma} = \frac{1}{V} \sum_{\mathbf{k}} \delta\rho_{\mathbf{k}} \\ &= \frac{1}{2\sqrt{4\pi}} \mathcal{N} \delta\rho_{00} = \frac{1}{2\sqrt{4\pi}} \mathcal{N} \frac{\delta\bar{\rho}_{00}}{1 + F_0^S} = \frac{1}{1 + F_0^S} \delta\bar{n}. \end{aligned}$$

The variation $\delta\bar{n}$ with respect to a variation of chemical potential is the same as for free particles with density of states \mathcal{N} , namely

$$\frac{\delta\bar{n}}{\delta\mu} = \mathcal{N}.$$

Therefore we finally obtain that

$$\kappa = \frac{1}{1 + F_0^S} \frac{\mathcal{N}}{\mathcal{N}^{(0)}} \kappa^{(0)}, \quad (1.30)$$

where $\kappa^{(0)}$ is the compressibility of the original free particles which have density of states $\mathcal{N}^{(0)}$.

Magnetic susceptibility

A magnetic field B , e.g. in the z -direction, introduces a Zeeman term in the Hamiltonian

$$\delta\mathcal{H} = -g \mu_B B \frac{1}{2} (N_{\uparrow} - N_{\downarrow}),$$

²Note that

$$Y_{00}(\Omega) = \sqrt{\frac{1}{4\pi}}.$$

where N_σ is the total number of spin- σ electrons, that acts as a difference of chemical potential for spin up and down electrons: $\delta\mu_\uparrow - \delta\mu_\downarrow = g\mu_B B$. Since the total magnetization is also conserved, the quasiparticles acquire the same difference in chemical potentials. The magnetization per unit volume δm can therefore be calculated by the quasiparticles through

$$\begin{aligned}\delta m &= g\mu_B \frac{1}{2V} \sum_{\mathbf{k}} \delta n_{\mathbf{k}\uparrow} - \delta n_{\mathbf{k}\downarrow} = g\mu_B \frac{1}{2V} \sum_{\mathbf{k}} \delta\sigma_{\mathbf{k}}^z = g\mu_B \frac{1}{4\sqrt{4\pi}} \mathcal{N} \delta\sigma_{00}^z \\ &= g\mu_B \frac{1}{4\sqrt{4\pi}} \mathcal{N} \frac{\delta\bar{\sigma}_{00}^z}{1 + F_0^A} = \frac{\delta\bar{m}}{1 + F_0^A}.\end{aligned}$$

Once again, since the local equilibrium magnetization $\delta\bar{m}$ is equivalent to the response of free particles with density of states \mathcal{N} , instead of \mathcal{N}_0 as for the original particles, we obtain that the magnetic susceptibility χ is

$$\chi = \frac{\delta m}{\delta B} = \frac{1}{1 + F_0^A} \frac{\mathcal{N}}{\mathcal{N}^{(0)}} \chi^{(0)}, \quad (1.31)$$

where $\chi^{(0)}$ is the susceptibility the original free-particles.

1.3 Quasiparticle transport equation

Let us suppose to perturb the Landau-Fermi liquid by an external probe that varies in space on a wavelength $1/q$ and in time on a period $1/\omega$. If

$$q \ll k_F, \quad \omega \ll \mu,$$

where k_F is the Fermi momentum ($\epsilon(k_F) = \mu$), the probe will affect only quasiparticles extremely close to the Fermi-sea. In this limit, we can safely adopt a semi-classical approach and introduce a space- and time-dependent density of quasiparticle occupation numbers at momentum $|\mathbf{k}| \sim k_F$

$$n_{\mathbf{k}\sigma}(\mathbf{x}, t),$$

and its space and time Fourier transform

$$n_{\mathbf{k}\sigma}(\mathbf{q}, \omega).$$

Fixing both coordinate \mathbf{x} and momentum \mathbf{k} is allowed in spite of the Heisenberg principle $\Delta x \Delta k \simeq 1$, because

$$\Delta k \simeq \frac{1}{\Delta x} \simeq q \ll k_F,$$

so that the quantum indeterminacy of momentum Δk is much smaller than its typical value k_F .

Since the quasiparticle occupation number is not a conserved quantity, its density should follow a Liouville equation

$$\frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial t} + \frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{x}} \frac{\partial \mathbf{x}}{\partial t} + \frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{k}} \frac{\partial \mathbf{k}}{\partial t} = I_{\mathbf{k}\sigma}(\mathbf{x}, t), \quad (1.32)$$

where $I_{\mathbf{k}\sigma}(\mathbf{x}, t)$ is a collision integral and corresponds to the transition rate within a volume $d\mathbf{x}$ around \mathbf{x} of all processes in which quasiparticles have a transition from any other state into (\mathbf{k}, σ) minus the transition rate of the inverse processes.

In the absence of the external probe, quasiparticles are at equilibrium and their density is uniform. Once the probe is applied, the density deviates from its uniform equilibrium value and acquires space and time dependence. In general the external force that acts on the real particles can not be identified with the force felt by the quasiparticles unless the external field couples to a conserved quantity. This is the case of a scalar potential coupled to the charge density, or a magnetic field that couples to the spin density. In those cases, the deviation from equilibrium of the energy becomes non-uniform hence can be generalized into

$$\begin{aligned} \delta E(t) &= \int d\mathbf{x} \delta E(\mathbf{x}, t) = \sum_{\mathbf{k}\sigma} \int d\mathbf{x} \left(\epsilon_{\mathbf{k}} + V_{\sigma}(\mathbf{x}, t) \right) \delta n_{\mathbf{k}\sigma}(\mathbf{x}, t) \\ &\quad + \frac{1}{2} \sum_{\mathbf{k}\mathbf{k}'} \sum_{\sigma\sigma'} \int d\mathbf{x} d\mathbf{y} \delta n_{\mathbf{k}\sigma}(\mathbf{x}, t) f_{\mathbf{k}\sigma \mathbf{k}'\sigma'}(\mathbf{x} - \mathbf{y}) \delta n_{\mathbf{k}'\sigma'}(\mathbf{y}, t), \end{aligned} \quad (1.33)$$

where $V_{\sigma}(\mathbf{x}, t)$ represents the action of the external probe, $V_{\uparrow} = V_{\downarrow}$ for a scalar potential and $V_{\uparrow} = -V_{\downarrow}$ for a magnetic field, and we assume that the quasiparticle interaction is instantaneous and only depends on the distance. The above expression provides also the proper definition of the quasiparticle excitation energy as

$$\bar{\epsilon}_{\mathbf{k}\sigma}(\mathbf{x}, t) = \epsilon_{\mathbf{k}} + V_{\sigma}(\mathbf{x}, t) + \sum_{\mathbf{k}'\sigma'} \int d\mathbf{y} f_{\mathbf{k}\sigma \mathbf{k}'\sigma'}(\mathbf{x} - \mathbf{y}) \delta n_{\mathbf{k}'\sigma'}(\mathbf{y}, t). \quad (1.34)$$

For neutral particles we can assume that

$$f_{\mathbf{k}\sigma \mathbf{k}'\sigma'}(\mathbf{x} - \mathbf{y}) = f_{\mathbf{k}\sigma \mathbf{k}'\sigma'} \delta(\mathbf{x} - \mathbf{y}),$$

in which case

$$\bar{\epsilon}_{\mathbf{k}\sigma}(\mathbf{x}, t) = \epsilon_{\mathbf{k}} + V_{\sigma}(\mathbf{x}, t) + \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma \mathbf{k}'\sigma'} \delta n_{\mathbf{k}'\sigma'}(\mathbf{x}, t). \quad (1.35)$$

By means of the Hamiltonian equations for conjugate variables

$$\frac{\partial \mathbf{x}}{\partial t} = \frac{\partial H}{\partial \mathbf{k}}, \quad \frac{\partial \mathbf{k}}{\partial t} = -\frac{\partial H}{\partial \mathbf{x}},$$

Eq. (1.32) can be finally written as

$$\frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial t} + \frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{x}} \frac{\partial \bar{\epsilon}_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{k}} - \frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{k}} \frac{\partial \bar{\epsilon}_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{x}} = I_{\mathbf{k}\sigma}(\mathbf{x}, t), \quad (1.36)$$

At linear order in the external probe $V_\sigma(\mathbf{x}, t)$, the occupation density

$$n_{\mathbf{k}\sigma}(\mathbf{x}, t) = n_{\mathbf{k}\sigma}^0 + \delta n_{\mathbf{k}\sigma}(\mathbf{x}, t),$$

and, consistently,

$$\bar{\epsilon}_{\mathbf{k}\sigma}(\mathbf{x}, t) = \epsilon_{\mathbf{k}} + \delta \epsilon_{\mathbf{k}\sigma}(\mathbf{x}, t),$$

where

$$\delta \epsilon_{\mathbf{k}\sigma}(\mathbf{x}, t) = \frac{\delta E}{\delta n_{\mathbf{k}\sigma}(\mathbf{x}, t)} - \epsilon_{\mathbf{k}} = V_\sigma(\mathbf{x}, t) + \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma \mathbf{k}'\sigma'} \delta n_{\mathbf{k}'\sigma'}(\mathbf{x}, t).$$

Consequently, the linearized transport equation (1.36) reads

$$\begin{aligned} & \frac{\partial \delta n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial t} + \frac{\partial \delta n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{x}} \frac{\partial \epsilon_{\mathbf{k}}}{\partial \mathbf{k}} - \frac{\partial n_{\mathbf{k}}^0}{\partial \mathbf{k}} \frac{\partial \delta \epsilon_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{x}} \\ &= \frac{\partial \delta n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial t} + \frac{\partial \delta n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{x}} \frac{\partial \epsilon_{\mathbf{k}}}{\partial \mathbf{k}} - \frac{\partial n_{\mathbf{k}}^0}{\partial \mathbf{k}} \left[\frac{\partial V_\sigma(\mathbf{x}, t)}{\partial \mathbf{x}} + \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma \mathbf{k}'\sigma'} \frac{\partial \delta n_{\mathbf{k}'\sigma'}(\mathbf{x}, t)}{\partial \mathbf{x}} \right] \\ &= \frac{\partial \delta n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial t} + \frac{\partial \delta n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{x}} \frac{\partial \epsilon_{\mathbf{k}}}{\partial \mathbf{k}} \\ &\quad - \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \frac{\partial \epsilon_{\mathbf{k}}}{\partial \mathbf{k}} \left[\frac{\partial V_\sigma(\mathbf{x}, t)}{\partial \mathbf{x}} + \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma \mathbf{k}'\sigma'} \frac{\partial \delta n_{\mathbf{k}'\sigma'}(\mathbf{x}, t)}{\partial \mathbf{x}} \right] \\ &= \frac{\partial \delta n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial t} + \mathbf{v}_{\mathbf{k}} \cdot \frac{\partial \delta n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{x}} \\ &\quad - \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \mathbf{v}_{\mathbf{k}} \cdot \left[\frac{\partial V_\sigma(\mathbf{x}, t)}{\partial \mathbf{x}} + \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma \mathbf{k}'\sigma'} \frac{\partial \delta n_{\mathbf{k}'\sigma'}(\mathbf{x}, t)}{\partial \mathbf{x}} \right] \\ &\equiv \frac{\partial \delta n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial t} + \mathbf{v}_{\mathbf{k}} \cdot \frac{\partial \delta n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{x}} + \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \mathbf{v}_{\mathbf{k}} \cdot \mathbf{F}_{\mathbf{k}\sigma}(\mathbf{x}, t) \\ &= I_{\mathbf{k}\sigma}(\mathbf{x}, t), \end{aligned} \quad (1.37)$$

where

$$\mathbf{v}_{\mathbf{k}} = \frac{\partial \epsilon_{\mathbf{k}}}{\partial \mathbf{k}}$$

is the quasiparticle group velocity. The Landau transport equation (1.37) resembles the conventional Boltzmann equation apart from the fact that the effective force $\mathbf{F}_{\mathbf{k}\sigma}(\mathbf{x}, t)$ depends self-consistently on the occupation density.

1.3.1 Quasiparticle current density

Let us set $V(\mathbf{x}, t) = 0$ in (1.37). We note that

$$\frac{1}{V} \sum_{\mathbf{k}\sigma} \delta n_{\mathbf{k}\sigma}(\mathbf{x}, t) = \delta\rho(\mathbf{x}, t),$$

where $\delta\rho(\mathbf{x}, t)$ is the deviation of the density with respect to the uniform equilibrium value, and moreover that

$$\frac{1}{V} \sum_{\mathbf{k}\sigma} I_{\mathbf{k}\sigma}(\mathbf{x}, t) = 0,$$

by particle conservation (recall the meaning of the collision integral $I_{\mathbf{k}\sigma}$). Through Eq. (1.37) and using the relation (1.29) between the deviations from global and local equilibrium, we find the following equation for the evolution of $\delta\rho(\mathbf{x}, t)$ in the absence of external probes:

$$\begin{aligned} \frac{\partial \delta\rho(\mathbf{x}, t)}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot \frac{1}{V} \sum_{\mathbf{k}\sigma} \mathbf{v}_k \left[\delta n_{\mathbf{k}\sigma}(\mathbf{x}, t) - \frac{\partial n_k^0}{\partial \epsilon_k} \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma\mathbf{k}'\sigma'} \delta n_{\mathbf{k}'\sigma'}(\mathbf{x}, t) \right] \\ = \frac{\partial \delta\rho(\mathbf{x}, t)}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot \frac{1}{V} \sum_{\mathbf{k}\sigma} \mathbf{v}_k \delta \bar{n}_{\mathbf{k}\sigma}(\mathbf{x}, t) = 0. \end{aligned} \quad (1.38)$$

Since the integral over the whole space of $\delta\rho(\mathbf{x}, t)$ is the variation of the total number of real particles, which is conserved, then $\delta\rho(\mathbf{x}, t)$ should also satisfy a continuity equation

$$\frac{\partial \delta\rho(\mathbf{x}, t)}{\partial t} + \frac{\partial \mathbf{J}(\mathbf{x}, t)}{\partial \mathbf{x}} = 0,$$

that allows to identify the current density $\mathbf{J}(\mathbf{x}, t)$ (note that, at equilibrium, the current is zero hence $\mathbf{J}(\mathbf{x}, t) = \delta\mathbf{J}(\mathbf{x}, t)$)

$$\begin{aligned} \mathbf{J}(\mathbf{x}, t) &= \frac{1}{V} \sum_{\mathbf{k}\sigma} \mathbf{v}_k \delta \bar{n}_{\mathbf{k}\sigma}(\mathbf{x}, t) \\ &= \frac{1}{V} \sum_{\mathbf{k}\sigma} \mathbf{v}_k \left[\delta n_{\mathbf{k}\sigma}(\mathbf{x}, t) - \frac{\partial n_k^0}{\partial \epsilon_k} \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma\mathbf{k}'\sigma'} \delta n_{\mathbf{k}'\sigma'}(\mathbf{x}, t) \right] \\ &= \frac{1}{V} \sum_{\mathbf{k}\sigma} \delta n_{\mathbf{k}\sigma}(\mathbf{x}, t) \left[\mathbf{v}_k - \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma\mathbf{k}'\sigma'} \frac{\partial n_{\mathbf{k}'\sigma'}^0}{\partial \epsilon_{\mathbf{k}'}} \mathbf{v}_{\mathbf{k}'} \right] \\ &\equiv \frac{1}{V} \sum_{\mathbf{k}\sigma} \delta n_{\mathbf{k}\sigma}(\mathbf{x}, t) \mathbf{J}_{\mathbf{k}\sigma}. \end{aligned} \quad (1.39)$$

This equation shows that the actual current matrix element $\mathbf{J}_{\mathbf{k}\sigma}$ is not the group velocity \mathbf{v}_k – the moving quasiparticle induces a flow of other quasiparticles because of their mutual interaction.

We observe that at very low temperature

$$\frac{\partial n_{\mathbf{k}'\sigma'}^0}{\partial \epsilon_{\mathbf{k}'}} = \frac{\partial f(\epsilon_{\mathbf{k}'} - \mu)}{\partial \epsilon_{\mathbf{k}'}} \simeq -\delta(\epsilon_{\mathbf{k}'} - \mu),$$

namely \mathbf{k}' lies on the Fermi surface. If the system is isotropic, then on the Fermi sphere

$$\mathbf{v}_{\mathbf{k}} = \frac{\partial \epsilon(|\mathbf{k}|)}{\partial \mathbf{k}} = v_F \frac{\mathbf{k}}{|\mathbf{k}|} = \frac{k_F}{m_*} \frac{\mathbf{k}}{|\mathbf{k}|},$$

with v_F and m_* the Fermi velocity and effective mass, respectively, of the quasiparticles. Using an expansion like (1.16) in terms of spherical harmonics we find that, for instance the z -component of the current density, J_z , is

$$\begin{aligned} J_z(\mathbf{x}, t) &= \frac{1}{V} \sum_{\mathbf{k}\sigma} (\mathbf{v}_{\mathbf{k}})_z \delta \bar{n}_{\mathbf{k}\sigma}(\mathbf{x}, t) \\ &= \frac{1}{V} \sum_{\mathbf{k}\sigma} v_F \frac{k_z}{|\mathbf{k}|} \delta(\epsilon_{\mathbf{k}} - \mu) \sum_{lm} Y_{lm}(\Omega_{\mathbf{k}}) \delta \bar{n}_{lm\sigma}(\mathbf{x}, t) \\ &= \frac{v_F}{2} \mathcal{N} \sum_{lm} \delta \bar{\rho}_{lm}(\mathbf{x}, t) \int \frac{d\Omega}{4\pi} \cos \theta Y_{lm}(\Omega) \\ &= \frac{v_F}{2\sqrt{12\pi}} \mathcal{N} \delta \bar{\rho}_{10}(\mathbf{x}, t) = \frac{v_F}{2\sqrt{12\pi}} \mathcal{N} \left(1 + \frac{F_1^S}{3}\right) \delta \rho_{10}(\mathbf{x}, t) \\ &= \frac{v_F}{v_F^{(0)}} \left(1 + \frac{F_1^S}{3}\right) \left[\frac{v_F^{(0)}}{2\sqrt{12\pi}} \mathcal{N} \delta \rho_{10}(\mathbf{x}, t) \right] \\ &= \frac{v_F}{v_F^{(0)}} \left(1 + \frac{F_1^S}{3}\right) \frac{1}{V} \sum_{\mathbf{k}\sigma} (\mathbf{v}_{\mathbf{k}}^{(0)})_z \delta n_{\mathbf{k}\sigma}(\mathbf{x}, t), \end{aligned} \quad (1.40)$$

where $\mathbf{v}_{\mathbf{k}}^{(0)}$ is the group velocity of the free particles on the Fermi surface

$$\mathbf{v}_{\mathbf{k}}^{(0)} = \frac{\partial \epsilon^{(0)}(|\mathbf{k}|)}{\partial \mathbf{k}} = v_F^{(0)} \frac{\mathbf{k}}{|\mathbf{k}|} = \frac{k_F}{m} \frac{\mathbf{k}}{|\mathbf{k}|}. \quad (1.41)$$

The x and y component can be found analogously and involve combinations of $\delta n_{1+1}(\mathbf{x}, t)$ and $\delta n_{1-1}(\mathbf{x}, t)$. Therefore in general it holds that

$$\begin{aligned} \mathbf{J}(\mathbf{x}, t) &= \frac{v_F}{v_F^{(0)}} \left(1 + \frac{F_1^S}{3}\right) \frac{1}{V} \sum_{\mathbf{k}\sigma} \mathbf{v}_{\mathbf{k}}^{(0)} \delta n_{\mathbf{k}\sigma}(\mathbf{x}, t) \\ &= \frac{m}{m_*} \left(1 + \frac{F_1^S}{3}\right) \frac{1}{V} \sum_{\mathbf{k}\sigma} \mathbf{v}_{\mathbf{k}}^{(0)} \delta n_{\mathbf{k}\sigma}(\mathbf{x}, t). \end{aligned} \quad (1.42)$$

As a concluding remark we notice that we could also follow the same analysis in connection with the spin-current density, the only difference being that F_1^S would be substituted by F_1^A .

Translationally invariant systems

In a system that is not only isotropic but also translationally invariant, the current matrix element is

$$\mathbf{J}_\mathbf{k} = \frac{\mathbf{k}}{m},$$

with m the mass of the real particles. Since the current is conserved, the total current per unit volume must be given in terms of quasiparticles by

$$J_z = \frac{1}{V} \sum_{\mathbf{k}\sigma} \frac{\mathbf{k}}{m} \delta n_{\mathbf{k}\sigma} = \frac{k_F}{2m\sqrt{12\pi}} \mathcal{N} \delta\rho_{10}. \quad (1.43)$$

Comparing (1.43) with (1.40) in the case in which the current density, hence the occupation density, are constant in time and space, i.e. $J_z(\mathbf{x}, t) = J_z$ and $\delta\rho_{10}(\mathbf{x}, t) = \delta\rho_{10}$, we conclude that, when translational invariance is unbroken, like in ${}^3\text{He}$, the following relation holds

$$\frac{m_*}{m} = 1 + \frac{F_1^S}{3}, \quad (1.44)$$

namely the effective mass and the Landau parameter F_1^S are not independent.

1.4 Collective excitations in the collisionless regime

The collision integral in the transport equation determines a typical collision time τ . If one is interested in phenomena that occur on a time scale smaller than τ , namely on frequencies $\omega \gg 1/\tau$, then the collision integral can be safely neglected and the transport equation (1.37) in frequency and momentum space becomes

$$(\omega - \mathbf{q} \cdot \mathbf{v}_\mathbf{k}) \delta n_{\mathbf{k}\sigma}(\mathbf{q}, \omega) + \mathbf{q} \cdot \mathbf{v}_\mathbf{k} \frac{\partial n_\mathbf{k}^0}{\partial \epsilon_\mathbf{k}} \left[V_\sigma(\mathbf{q}, \omega) + \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma} f_{\mathbf{k}'\sigma'} \delta n_{\mathbf{k}'\sigma'}(\mathbf{q}, \omega) \right] = 0. \quad (1.45)$$

The solution of this equation in the absence of external field gives information about the collective excitations of the quasiparticle gas. These excitations can also be thought as collective vibrations of the Fermi sphere. From this point of view, let us suppose that, along the direction identified by the Euler angles (θ, ϕ) , the z -axis being directed along the momentum \mathbf{q} , the Fermi momentum $\mathbf{k}_F = k_F (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$ for a spin σ quasiparticle changes into

$$\mathbf{k}_{F\sigma} = \left(k_F + u_\sigma(\theta, \phi) \right) (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta),$$

as if

$$k_{F\sigma}(\theta, \phi) = k_F \rightarrow k_{F\sigma}(\theta, \phi) = k_F + \delta k_F(\theta, \sigma) = k_F + u_\sigma(\theta, \phi).$$

The occupation number for a spin σ quasiparticle with momentum $\mathbf{k} = k (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$ changes accordingly as

$$n_{\mathbf{k}\sigma} = n_{\mathbf{k}\sigma}^0 \simeq \theta (k - k_{F\sigma}(\theta, \phi)) \rightarrow n_{\mathbf{k}\sigma} = n_{\mathbf{k}\sigma}^0 - \frac{\partial n_{\mathbf{k}}^0}{\partial \mathbf{k}} \delta \mathbf{k}_F = n_{\mathbf{k}\sigma}^0 + \delta n_{\mathbf{k}\sigma}.$$

We note that

$$\begin{aligned} \delta n_{\mathbf{k}\sigma} &= -\frac{\partial n_{\mathbf{k}}^0}{\partial \mathbf{k}} \delta \mathbf{k}_F \\ &= -\frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \frac{\partial \epsilon_{\mathbf{k}}}{\partial \mathbf{k}} \delta \mathbf{k}_F = -\frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} v_F u_\sigma(\theta, \phi). \end{aligned} \quad (1.46)$$

Inserting (1.46) into (1.45) with $V = 0$ we get

$$(\omega - v_F q \cos \theta) u_\sigma(\theta, \phi) + v_F q \cos \theta \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma \mathbf{k}'\sigma'} \frac{\partial n_{\mathbf{k}'\sigma'}^0}{\partial \epsilon_{\mathbf{k}'}} u_{\sigma'}(\theta', \phi') = 0. \quad (1.47)$$

For small vibrations of the Fermi sphere, we can assume that $f_{\mathbf{k}\sigma \mathbf{k}'\sigma'}$ only depends on the angle between \mathbf{k} and \mathbf{k}' , $f_{\mathbf{k}\sigma \mathbf{k}'\sigma'} = f_{\sigma\sigma'}(\theta_{\mathbf{k}\mathbf{k}'})$, their modula being equal to the equilibrium value of the Fermi momentum k_F . We note that, since

$$\frac{\partial n_{\mathbf{k}'\sigma'}^0}{\partial \epsilon_{\mathbf{k}'}} \simeq -\delta(\epsilon(|\mathbf{k}'|) - \mu),$$

it follows that

$$\begin{aligned} \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma \mathbf{k}'\sigma'} \frac{\partial n_{\mathbf{k}'\sigma'}^0}{\partial \epsilon_{\mathbf{k}'}} u_{\sigma'}(\theta', \phi') &= -2V \int \frac{4\pi |\mathbf{k}'|^2 d|\mathbf{k}'|}{(2\pi)^3} \delta(\epsilon(|\mathbf{k}'|) - \mu) \\ &\times \frac{1}{2} \int \frac{d\Omega_{\mathbf{k}'}}{4\pi} f_{\sigma\sigma'}(\theta_{\mathbf{k}\mathbf{k}'}) u_{\sigma'}(\Omega_{\mathbf{k}'}) \\ &= -V \mathcal{N} \frac{1}{2} \int \frac{d\Omega_{\mathbf{k}'}}{4\pi} f_{\sigma\sigma'}(\theta_{\mathbf{k}\mathbf{k}'}) u_{\sigma'}(\Omega_{\mathbf{k}'}) = -\frac{1}{2} \int \frac{d\Omega_{\mathbf{k}'}}{4\pi} F_{\sigma\sigma'}(\theta_{\mathbf{k}\mathbf{k}'}) u_{\sigma'}(\Omega_{\mathbf{k}'}), \end{aligned}$$

where, generalizing Eq. (1.22), the F -parameters are defined through

$$F_{\sigma\sigma'}(\theta_{\mathbf{k}\mathbf{k}'}) = V \mathcal{N} f_{\sigma\sigma'}(\theta_{\mathbf{k}\mathbf{k}'}).$$

If furtermore we define, for spin-isotropic models,

$$u^S = u_\uparrow + u_\downarrow, \quad u^A = u_\uparrow - u_\downarrow,$$

$$F_{\uparrow\uparrow} = F_{\downarrow\downarrow} = F^S + F^A, \quad F_{\uparrow\downarrow} = F_{\downarrow\uparrow} = F^S - F^A,$$

we find, defining $\lambda = \omega/v_F q$, the following equation

$$(\lambda - \cos \theta_{\mathbf{k}}) u^{S(A)}(\theta_{\mathbf{k}}, \phi_{\mathbf{k}}) - \cos \theta \int \frac{d\Omega_{\mathbf{k}'}}{4\pi} F^{S(A)}(\theta_{\mathbf{kk}'}) u^{S(A)}(\theta_{\mathbf{k}'}, \phi_{\mathbf{k}'}) = 0. \quad (1.48)$$

We write, dropping the indices S and A ,

$$\begin{aligned} u(\theta, \phi) &= \sum_{lm} Y_{lm}(\theta, \phi) u_{lm}, \\ F(\theta_{\mathbf{kk}'}) &= \sum_l P_l(\theta_{\mathbf{kk}'}) F_l, \end{aligned}$$

so that Eq. (1.48) can be re-written as

$$\sum_{lm} Y_{lm}(\theta_{\mathbf{k}}, \phi_{\mathbf{k}}) u_{lm} \left[(\lambda - \cos \theta_{\mathbf{k}}) - \frac{\cos \theta_{\mathbf{k}}}{2l+1} F_l \right] = 0. \quad (1.49)$$

Since

$$\cos \theta = \sqrt{\frac{4\pi}{3}} Y_{10}(\theta, \phi),$$

l is not a good quantum number of Eq. (1.49), while m is. In particular $m = 0$ corresponds to longitudinal vibrations of the Fermi sphere, $m = 1$ to dipolar vibrations and $m = 2$ to quadrupolar ones. We observe that a solution of (1.49) at $\omega = 0$ would imply that a deformation of the Fermi sphere would be cost-free, namely that the Fermi sphere is unstable. At $\lambda = 0$, l is a good quantum number, so that a $\lambda = 0$ solution of (1.49) occurs whenever there is a value of l such that, see Eq. (1.23),

$$1 + \frac{F_l^{S(A)}}{2l+1} = 0 = \frac{F_l^{S(A)}}{A_l^{S(A)}}, \quad (1.50)$$

which is the condition for the instability of the Landau-Fermi liquid. We note that, since $F_l^{S(A)}$ is generally non zero, the instability implies a singularity of the Landau A -parameters.

1.4.1 Zero sound

Let us assume, as commonly done, that only $F_0^{S(A)}$ and $F_1^{S(A)}$ are not negligible, and study Eq. (1.49) for longitudinal vibrations, $m = 0$. In this case, dropping for simplicity the labels S and A , we obtain

$$(\lambda - \cos \theta) u(\theta) = \sum_{lm} (\lambda - \cos \theta) Y_{lm}(\theta_{\mathbf{k}}, \phi_{\mathbf{k}}) u_{lm} = \cos \theta F_0 Y_{00} u_{00} + \frac{\cos \theta}{3} F_1 Y_{10} u_{10}. \quad (1.51)$$

We define,

$$C = \sqrt{\frac{1}{4\pi}} F_0 u_{00}, \quad (1.52)$$

$$D = \frac{1}{3} \sqrt{\frac{3}{4\pi}} F_1 u_{10}, \quad (1.53)$$

and, by noting that

$$Y_{00} = \sqrt{\frac{1}{4\pi}}, \quad \cos \theta = \sqrt{\frac{4\pi}{3}} Y_{10},$$

we get the formal solution

$$u(\theta) = \frac{C \cos \theta + D \cos^2 \theta}{\lambda - \cos \theta}. \quad (1.54)$$

In terms of this solution

$$\begin{aligned} \sqrt{\frac{1}{4\pi}} u_{00} &= \int \frac{d\Omega}{4\pi} \frac{C \cos \theta + D \cos^2 \theta}{\lambda - \cos \theta} \\ &= C I_1 + D I_2, \end{aligned} \quad (1.55)$$

$$\begin{aligned} \frac{1}{3} \sqrt{\frac{3}{4\pi}} u_{10} &= \int \frac{d\Omega}{4\pi} \cos \theta \frac{C \cos \theta + D \cos^2 \theta}{\lambda - \cos \theta} \\ &= C I_2 + D I_3, \end{aligned} \quad (1.56)$$

where

$$I_n = \int_{-1}^1 \frac{dz}{2} \frac{z^n}{\lambda - z}. \quad (1.57)$$

Therefore the self-consistency condition that has to be satisfied is

$$C = F_0 (C I_1 + D I_2), \quad (1.58)$$

$$D = F_1 (C I_2 + D I_3), \quad (1.59)$$

which have a solution if

$$1 = F_0 \left(I_1 + F_1 \frac{I_2^2}{1 - F_1 I_3} \right) \quad (1.60)$$

By realizing that

$$I_1 = -1 + \frac{\lambda}{2} \ln \left(\frac{\lambda+1}{\lambda-1} \right),$$

$$I_2 = \lambda I_1,$$

$$I_3 = -\frac{1}{3} + \lambda^2 I_1,$$

we finally get that (1.60) is satisfied if

$$1 = (F_0 + \lambda^2 A_1) I_1, \quad (1.61)$$

where, by definition,

$$A_1 = \frac{F_1}{1 + F_1/3}.$$

We note that, for $\lambda \leq 1$,

$$I_1 \simeq -1 + \lambda^2 - i \frac{\pi}{2} \lambda,$$

has a finite imaginary part. This implies that the frequency ω that solves (1.61) is necessarily complex, hence that it does not correspond to a stable collective mode but rather to a damped one. Therefore the only stable solutions of (1.61) must correspond to $\lambda \geq 1$.

For $\lambda \simeq 1 + \delta\lambda$, with $0 < \delta\lambda \ll 1$,

$$I_1 \simeq -\frac{1}{2} \ln \frac{e^2 \delta\lambda}{2},$$

leading to

$$\delta\lambda \simeq 2 \exp \left[-2 \left(1 + \frac{1}{F_0 + A_1} \right) \right]. \quad (1.62)$$

which is consistent with the assumption $\delta\lambda \ll 1$ only if

$$0 \leq F_0 + A_1 \ll 1.$$

In other words, when the Landau parameters are positive and very small, the stable collective modes propagate like sound modes with a velocity

$$v \simeq v_F \left(1 + 2 \exp \left[-2 \left(1 + \frac{1}{F_0 + A_1} \right) \right] \right),$$

slightly larger than the Fermi velocity. These modes correspond to a deformation of the Fermi sphere of the form

$$u(\theta) \simeq \frac{C \cos \theta + D \cos^2 \theta}{1 - \cos \theta + \delta\lambda},$$

that are strongly peaked to $\theta = 0$, namely in the direction of the propagating wave-vector \mathbf{q} .

In the opposite case of $\lambda \gg 1$,

$$I_1 \simeq \frac{1}{3\lambda^2} + \frac{1}{5\lambda^4},$$

and the solution of (1.60) is readily found to be

$$\lambda^2 = \frac{\omega^2}{v_F^2 q^2} = \left(\frac{F_0}{3} + \frac{A_1}{5} \right) \left(1 + \frac{F_1}{3} \right), \quad (1.63)$$

that requires the right hand side to be positive and much greater than one. Again this solution describes collective modes that propagate acoustically with a velocity this time much bigger than v_F and that correspond to a deformation of the form

$$u(\theta) \simeq \frac{C \cos \theta + D \cos^2 \theta}{\lambda},$$

that involves the whole Fermi sphere.

These collective modes that may emerge in the collisionless regime and propagate like sound modes were called by Landau “zero sounds”, as opposed to the first sound that exists in the collision regime. The existence of these new modes of a Landau-Fermi liquid depends on the quasiparticle interaction parameters F , that act as a restoring force absent for non-interacting electrons. Usually, for repulsive interactions, F_0^S is positive and F_0^A negative, while $A_1^{S(A)}$ is negligible.³ In this case only charge zero-sound, i.e. a Fermi-sphere deformation in the channel

$$u^S = u_\uparrow + u_\downarrow,$$

is a stable collective mode, while a spin zero-sound in the channel

$$u^A = u_\uparrow - u_\downarrow,$$

is not.

1.5 Collective excitations in the collision regime: first sound

For frequencies much smaller than the typical collision rate, the collision integral can not be neglected anymore and, as a result, any deformation of the Fermi sphere is destined to decay. The only exceptions are those excitations that correspond in the limit $q \rightarrow 0$ to conserved

³For repulsive interaction, the effective mass m_* increases with respect to the non-interacting system – the quasiparticles move more slowly than free ones. Furthermore, the magnetic susceptibility increases even more, since the slowed down quasiparticles with opposite spin repel each other, hence can react quite efficiently to a magnetic field. On the contrary, the compressibility κ decreases, as adding particles costs more energy. Since

$$\frac{\kappa}{\kappa^{(0)}} = \frac{m_*}{m} \frac{1}{1 + F_0^S}, \quad \frac{\chi}{\chi^{(0)}} = \frac{m_*}{m} \frac{1}{1 + F_0^A},$$

it follows that $F_0^S > -1 + m_*/m > 0$ and $F_0^A \leq 0$.

quantities, in particular to charge and momentum densities, in which case it is guaranteed that $\sum_{\mathbf{k}\sigma} I_{\mathbf{k}\sigma} = \sum_{\mathbf{k}\sigma} \mathbf{k} I_{\mathbf{k}\sigma} = 0$. Charge and momentum density excitations correspond to deformations of the Fermi sphere in the symmetric S -channel and with angular momenta $l = 0$ and $l = 1$, respectively, and $m = 0$. Through Eq. (1.49), the excitations in this regime satisfy the equation

$$0 = (\cos \theta - \lambda) Y_{00}(\Omega) u_{00} + (\cos \theta - \lambda) Y_{10}(\Omega) u_{10} + F_0^S \cos \theta Y_{00}(\Omega) u_{00} + F_1^S \cos \theta Y_{10}(\Omega) u_{10}. \quad (1.64)$$

Note that this equation differs from Eq. (1.51) for the zero sound because in that case F_0 and F_1 are assumed to be non-zero, but the $u(\theta)$ solving the equation has all l -components, unlike in this case. To solve (1.64), we multiply both sides once by $Y_{00}(\Omega)$ and integrate over the solid angle Ω , and do the same multiplying by $Y_{10}(\Omega)$, thus obtaining the following set of equations:

$$\begin{aligned} -\lambda u_{00} + \sqrt{\frac{1}{3}} \left(1 + \frac{F_1^S}{3} \right) u_{10} &= 0, \\ \sqrt{\frac{1}{3}} \left(1 + F_0^S \right) u_{00} - \lambda u_{10} &= 0. \end{aligned}$$

This set of equations has solution if

$$\lambda^2 = \frac{\omega^2}{v_F^2 q^2} = \frac{1}{3} \left(1 + F_0^S \right) \left(1 + \frac{F_1^S}{3} \right), \quad (1.65)$$

which corresponds to acoustic waves propagating with velocity s , where

$$s^2 = v_F^2 \left(1 + F_0^S \right) \left(1 + \frac{F_1^S}{3} \right). \quad (1.66)$$

One can readily realize that this is the ordinary sound velocity compatible with thermodynamics. Indeed, when local thermodynamic equilibrium is enforced by collisions - the hydrodynamic regime - the equations of motion for the charge density, $\rho(\mathbf{x}, t)$, through the continuity equation, and for the velocity field through the pressure $P(\mathbf{x}, t)$,⁴

$$\begin{aligned} \frac{\partial \rho(\mathbf{x}, t)}{\partial t} &= -n \frac{m}{m_*} \left(1 + \frac{F_1^S}{3} \right) \boldsymbol{\nabla} \cdot \mathbf{v}(\mathbf{x}, t) \\ m n \frac{\partial \mathbf{v}(\mathbf{x}, t)}{\partial t} &= -\boldsymbol{\nabla} P(\mathbf{x}, t), \end{aligned}$$

⁴We assume that the particle velocity field is related to the current as in Eq. (1.42), where by definition

$$n \mathbf{v}(\mathbf{x}, t) = \frac{1}{V} \sum_{\mathbf{k}\sigma} \mathbf{v}_{\mathbf{k}}^{(0)} \delta n_{\mathbf{k}\sigma}(\mathbf{x}, t).$$

with n the average density, can be solved using the thermodynamic relation

$$\delta P(\mathbf{x}, t) = \frac{\partial P}{\partial \rho} \delta \rho(\mathbf{x}, t) = \frac{1}{n \kappa} \delta \rho(\mathbf{x}, t),$$

where κ is the thermodynamic compressibility. The solution gives ordinary sound with a velocity that coincides with (1.66).

1.6 Linear response functions

An external field induces deviations of the quasiparticle occupation numbers, and the linear relation between these deviations and the field responsible for them are the so-called “linear response functions”. Let us go back to the transport equation (1.37), and assume in what follows that the collision integral is negligible. After space and time Fourier transform, Eq. (1.37) is⁵

$$\begin{aligned} & (\mathbf{q} \cdot \mathbf{v}_\mathbf{k} - \omega) \delta n_{\mathbf{k}\sigma}(\mathbf{q}, \omega) - \mathbf{q} \cdot \mathbf{v}_\mathbf{k} \frac{\partial n_\mathbf{k}^0}{\partial \epsilon_\mathbf{k}} \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma \mathbf{k}'\sigma'} \delta n_{\mathbf{k}'\sigma'}(\mathbf{q}, \omega) \\ &= \mathbf{q} \cdot \mathbf{v}_\mathbf{k} \frac{\partial n_\mathbf{k}^0}{\partial \epsilon_\mathbf{k}} V_\sigma(\mathbf{q}, \omega). \end{aligned} \quad (1.67)$$

We stress once more that the external field that enters this equation can be identified with the actual field acting on the true particles only if it refers to conserved quantities, hence the charge, in which case

$$V_\sigma(\mathbf{q}, \omega) = V(\mathbf{q}, \omega), \quad (1.68)$$

and the spin,

$$V_\uparrow(\mathbf{q}, \omega) = -V_\downarrow(\mathbf{q}, \omega). \quad (1.69)$$

⁵ In deriving the transport equation we assume implicitly the system to be initially, for instance at time $t \rightarrow -\infty$, at equilibrium. This implies that the external field that moves away from equilibrium must initially be absent, i.e. $V(\mathbf{x}, t \rightarrow -\infty) \rightarrow 0$. A simple and convenient choice is to represent, for all times before the measure, performed e.g. at $t = 0$, an external field that oscillates with frequency ω as

$$V(\mathbf{x}, t) = V(\mathbf{x}, \omega) e^{-i \omega t + \eta t},$$

with η an infinitesimal positive number. Consequently, the response of the system must follow the same time behavior, i.e.

$$\delta n_{\mathbf{k}\sigma}(\mathbf{x}, t) = \delta n_{\mathbf{k}\sigma}(\mathbf{x}, \omega) e^{-i \omega t + \eta t},$$

so that the time dependence cancels out from (1.37). When taking the time derivative,

$$\frac{\partial \delta n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial t} = -i(\omega + i\eta) \delta n_{\mathbf{k}\sigma}(\mathbf{x}, \omega) e^{-i \omega t + \eta t},$$

which implies that the frequency ω has to be interpreted in whatever follows as $\omega + i\eta$.

Let us write

$$\delta n_{\mathbf{k}\sigma}(\mathbf{q}, \omega) = -\frac{\mathbf{q} \cdot \mathbf{v}_\mathbf{k}}{\mathbf{q} \cdot \mathbf{v}_\mathbf{k} - \omega} \frac{\partial n_\mathbf{k}^0}{\partial \epsilon_\mathbf{k}} X_{\mathbf{k}\sigma}(\mathbf{q}, \omega), \quad (1.70)$$

through which Eq. (1.67) transforms into

$$\begin{aligned} X_{\mathbf{k}\sigma}(\mathbf{q}, \omega) &= \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma \mathbf{k}'\sigma'} \frac{\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}'}}{\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}'} - \omega} \frac{\partial n_{\mathbf{k}'}^0}{\partial \epsilon_{\mathbf{k}'}} X_{\mathbf{k}'\sigma'} \\ &= -V_\sigma(\mathbf{q}, \omega). \end{aligned} \quad (1.71)$$

1.6.1 Formal solution

Let us write Eq. (1.71) in matricial way like

$$[\hat{I} - \hat{f} \hat{K}] \vec{X} = -\vec{V}, \quad (1.72)$$

where the matrices have matrix elements

$$\begin{aligned} I_{\mathbf{k}\sigma \mathbf{k}'\sigma'} &= \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'}, \\ f_{\mathbf{k}\sigma \mathbf{k}'\sigma'} &= f_{\mathbf{k}\sigma \mathbf{k}'\sigma'}, \\ K_{\mathbf{k}\sigma \mathbf{k}'\sigma'} &= \frac{\mathbf{q} \cdot \mathbf{v}_\mathbf{k}}{\mathbf{q} \cdot \mathbf{v}_\mathbf{k} - \omega} \frac{\partial n_\mathbf{k}^0}{\partial \epsilon_\mathbf{k}} \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'}, \end{aligned}$$

and the vectors \vec{X} and \vec{V}

$$\begin{aligned} (\vec{X})_{\mathbf{k}\sigma} &= X_{\mathbf{k}\sigma}(\mathbf{q}, \omega), \\ (\vec{V})_{\mathbf{k}\sigma} &= V_\sigma(\mathbf{q}, \omega). \end{aligned}$$

The formal solution of (1.72) is

$$\vec{X} = -[\hat{I} - \hat{f} \hat{K}]^{-1} \vec{V}. \quad (1.73)$$

Let us suppose to introduce another matrix \hat{A} , with elements

$$(\hat{A})_{\mathbf{k}\sigma \mathbf{k}'\sigma'} = A_{\mathbf{k}\sigma \mathbf{k}'\sigma'}(\mathbf{q}, \omega), \quad (1.74)$$

that satisfies the set of equations

$$[\hat{I} - \hat{f} \hat{K}] \hat{A} = \hat{f}. \quad (1.75)$$

One readily derives from this equation that

$$\hat{A} = [\hat{I} - \hat{f} \hat{K}]^{-1} \hat{f},$$

hence that

$$\begin{aligned}\hat{A} \hat{K} &= [\hat{I} - \hat{f} \hat{K}]^{-1} \hat{f} \hat{K} = [\hat{I} - \hat{f} \hat{K}]^{-1} [\hat{f} \hat{K} - \hat{I} + \hat{I}] \\ &= -\hat{I} + [\hat{I} - \hat{f} \hat{K}]^{-1}.\end{aligned}$$

In other words

$$[\hat{I} - \hat{f} \hat{K}]^{-1} = \hat{A} \hat{K} + \hat{I}, \quad (1.76)$$

so that

$$\vec{X} = -[\hat{I} + \hat{A} \hat{K}] \vec{V},$$

that explicitly means

$$X_{\mathbf{k}\sigma}(\mathbf{q}, \omega) = -\sum_{\mathbf{k}'\sigma'} \left[\delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'} + A_{\mathbf{k}\sigma \mathbf{k}'\sigma'}(\mathbf{q}, \omega) \frac{\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}'}}{\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}'} - \omega} \frac{\partial n_{\mathbf{k}'}^0}{\partial \epsilon_{\mathbf{k}'}} \right] V_{\sigma'}(\mathbf{q}, \omega), \quad (1.77)$$

hence that

$$\delta n_{\mathbf{k}\sigma}(\mathbf{q}, \omega) = \frac{\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}}}{\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}} - \omega} \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \sum_{\sigma'} \left[\delta_{\sigma\sigma'} + \sum_{\mathbf{k}'} A_{\mathbf{k}\sigma \mathbf{k}'\sigma'}(\mathbf{q}, \omega) \frac{\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}'}}{\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}'} - \omega} \frac{\partial n_{\mathbf{k}'}^0}{\partial \epsilon_{\mathbf{k}'}} \right] V_{\sigma'}(\mathbf{q}, \omega), \quad (1.78)$$

that is the formal solution of (1.67). The functions $A_{b\mathbf{k}\sigma \mathbf{k}'\sigma'}(\mathbf{q}, \omega)$ are the so-called quasiparticle scattering amplitudes. We define as usual

$$\begin{aligned}A_{\mathbf{k}\sigma \mathbf{k}'\sigma}(\mathbf{q}, \omega) &= A_{\mathbf{k}\mathbf{k}'}^S(\mathbf{q}, \omega) + A_{\mathbf{k}\mathbf{k}'}^A(\mathbf{q}, \omega), \\ A_{\mathbf{k}\sigma \mathbf{k}'\sigma'}(\mathbf{q}, \omega) &= A_{\mathbf{k}\mathbf{k}'}^S(\mathbf{q}, \omega) - A_{\mathbf{k}\mathbf{k}'}^A(\mathbf{q}, \omega),\end{aligned}$$

with $\sigma \neq \sigma'$. We also introduce a vertex λ_σ that, in case of a scalar potential $V_\sigma(\mathbf{q}, \omega) = V(\mathbf{q}, \omega)$, is defined as

$$\lambda_\sigma = 1,$$

while it is

$$\lambda_\sigma = \delta_{\sigma\uparrow} - \delta_{\sigma\downarrow},$$

for a Zeeman-splitting magnetic field

$$V_\sigma(\mathbf{q}, \omega) = V(\mathbf{q}, \omega) \left(\delta_{\sigma\uparrow} - \delta_{\sigma\downarrow} \right) = V(\mathbf{q}, \omega) \lambda_\sigma.$$

Upon multiplying both sides of (1.78) by the corresponding vertex and summing over \mathbf{k} and σ and dividing by the volume, we find that the charge, $\delta\rho(\mathbf{q}, \omega)$, and spin, $\delta\sigma(\mathbf{q}, \omega)$, density deviations at linear order in the corresponding fields are given by

$$\delta\rho(\mathbf{q}, \omega) = \chi^S(\mathbf{q}, \omega) V(\mathbf{q}, \omega)$$

$$\delta\sigma(\mathbf{q}, \omega) = \chi^A(\mathbf{q}, \omega) V(\mathbf{q}, \omega),$$

where

$$\chi^{S(A)}(\mathbf{q}, \omega) = \frac{2}{V} \sum_{\mathbf{k}} \frac{\mathbf{q} \cdot \mathbf{v}_k}{\mathbf{q} \cdot \mathbf{v}_k - \omega} \frac{\partial n_k^0}{\partial \epsilon_k} \left[1 + 2 \sum_{\mathbf{k}'} A_{\mathbf{k}\mathbf{k}'}^{(S(A))}(\mathbf{q}, \omega) \frac{\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}'}}{\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}'} - \omega} \frac{\partial n_{\mathbf{k}'}^0}{\partial \epsilon_{\mathbf{k}'}} \right]. \quad (1.79)$$

Thus $-\chi^S(\mathbf{q}, \omega)$ is the dynamical compressibility $\kappa(\mathbf{q}, \omega)$, while $-\chi^A(\mathbf{q}, \omega)$ dynamical spin-susceptibility.

Limiting cases

We readily realize that, if $q = 0$ and $\omega \neq 0$, then the matrix $\hat{K} = 0$. In this case $\hat{A} = \hat{f}$, namely

$$A_{\mathbf{k}\sigma \mathbf{k}'\sigma'}(0, \omega) = f_{\mathbf{k}\sigma \mathbf{k}'\sigma'}. \quad (1.80)$$

In the opposite limit, $q \neq 0$ and $\omega = 0$, Eq. (1.75) reads explicitly

$$A_{\mathbf{k}\sigma \mathbf{k}'\sigma'}(\mathbf{q}, 0) - \sum_{\mathbf{p}\alpha} f_{\mathbf{k}\sigma \mathbf{p}\alpha} \frac{\partial n_{\mathbf{p}}^0}{\partial \epsilon_{\mathbf{p}}} A_{\mathbf{p}\alpha \mathbf{k}'\sigma'}(\mathbf{q}, 0) = f_{\mathbf{p}\alpha \mathbf{k}'\sigma'},$$

showing that $A_{\mathbf{k}\sigma \mathbf{k}'\sigma'}(\mathbf{q}, 0)$ is independent on \mathbf{q} . By writing

$$V \mathcal{N} A_{\mathbf{k}\sigma \mathbf{k}'\sigma'}(\mathbf{q}, 0) = \sum_l P_l(\theta_{\mathbf{k}\mathbf{k}'}) [A_l^S \pm A_l^A],$$

where the + sign refers to $\sigma = \sigma'$ and the - one otherwise, one readily recognize that A_l^S and A_l^A coincide with the Landau A -parameters of Eq. (1.23).

1.6.2 Low frequency limit of the response functions

For frequencies $\omega \ll v_F q$, we can expand $A_{\mathbf{k}\sigma \mathbf{k}'\sigma'}(\mathbf{q}, \omega)$ as

$$A_{\mathbf{k}\sigma \mathbf{k}'\sigma'}(\mathbf{q}, \omega) = A_{\mathbf{k}\sigma \mathbf{k}'\sigma'}(\mathbf{q}, 0) + \delta A_{\mathbf{k}\sigma \mathbf{k}'\sigma'}(\mathbf{q}, \omega), \quad (1.81)$$

where δA vanishes linearly at $\omega = 0$. We note that

$$\frac{\mathbf{q} \cdot \mathbf{v}_k}{\mathbf{q} \cdot \mathbf{v}_k - \omega} = 1 + \frac{\omega}{\mathbf{q} \cdot \mathbf{v}_k},$$

so that the linear variation δA has to satisfy the equation

$$\delta A_{\mathbf{k}\sigma \mathbf{k}'\sigma'}(\mathbf{q}, \omega) - \sum_{\mathbf{p}\alpha} f_{\mathbf{k}\sigma \mathbf{p}\alpha} \frac{\partial n_{\mathbf{p}}^0}{\partial \epsilon_{\mathbf{p}}} \delta A_{\mathbf{p}\alpha \mathbf{k}'\sigma'}(\mathbf{q}, \omega) = \sum_{\mathbf{p}\alpha} f_{\mathbf{k}\sigma \mathbf{p}\alpha} \frac{\partial n_{\mathbf{p}}^0}{\partial \epsilon_{\mathbf{p}}} \frac{\omega}{\mathbf{q} \cdot \mathbf{v}_{\mathbf{p}}} A_{\mathbf{p}\alpha \mathbf{k}'\sigma'}(\mathbf{q}, 0). \quad (1.82)$$

The integral over $\Omega_{\mathbf{p}}$ of the function $(\mathbf{q} \cdot \mathbf{v}_{\mathbf{p}})^{-1}$ is singular, hence we need some regularization. Indeed, as discussed in the footnote [5], the frequency ω above is actually $\omega + i\eta$, with η an infinitesimally small positive number. Therefore

$$\frac{\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}}}{\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}} - \omega} \rightarrow \frac{\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}}}{\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}} - \omega - i\eta} = 1 + \frac{\omega}{\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}} - i\eta} \simeq 1 + i\pi \delta(\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}}) + \mathcal{P} \frac{\omega}{\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}}},$$

where \mathcal{P} indicates the principal value. Therefore, within the S and A channels, Eq. (1.82) becomes (the principal value averages to zero hence does not contribute)

$$\delta A_{\mathbf{k}\mathbf{k}'}^{S(A)}(\mathbf{q}, \omega) - 2 \sum_{\mathbf{p}} f_{\mathbf{k}\mathbf{p}}^{S(A)} \frac{\partial n_{\mathbf{p}}^0}{\partial \epsilon_{\mathbf{p}}} \delta A_{\mathbf{p}\mathbf{k}'}^{S(A)}(\mathbf{q}, \omega) = 2\pi i \omega \sum_{\mathbf{p}} f_{\mathbf{k}\mathbf{p}}^{S(A)} \frac{\partial n_{\mathbf{p}}^0}{\partial \epsilon_{\mathbf{p}}} \delta(\mathbf{q} \cdot \mathbf{v}_{\mathbf{p}}) A_{\mathbf{p}\mathbf{k}'}^{S(A)}(\mathbf{q}, 0). \quad (1.83)$$

At first order in ω , Eq. (1.79) becomes (we drop the indices S and A)

$$\begin{aligned} \chi(\mathbf{q}, \omega) &\simeq \frac{2}{V} \sum_{\mathbf{k}} \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \left[1 + 2 \sum_{\mathbf{k}'} A_{\mathbf{k}\mathbf{k}'}(\mathbf{q}, 0) \frac{\partial n_{\mathbf{k}'}^0}{\partial \epsilon_{\mathbf{k}'}} \right] \\ &+ 2\pi i \omega \frac{1}{V} \sum_{\mathbf{k}} \delta(\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}}) \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \left[1 + 2 \sum_{\mathbf{k}'} A_{\mathbf{k}\mathbf{k}'}(\mathbf{q}, 0) \frac{\partial n_{\mathbf{k}'}^0}{\partial \epsilon_{\mathbf{k}'}} \right] \\ &+ 4\pi i \omega \frac{1}{V} \sum_{\mathbf{k}\mathbf{k}'} \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \frac{\partial n_{\mathbf{k}'}^0}{\partial \epsilon_{\mathbf{k}'}} A_{\mathbf{k}\mathbf{k}'}(\mathbf{q}, 0) \delta(\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}'}) \\ &+ 4 \frac{1}{V} \sum_{\mathbf{k}\mathbf{k}'} \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \frac{\partial n_{\mathbf{k}'}^0}{\partial \epsilon_{\mathbf{k}'}} \delta A_{\mathbf{k}\mathbf{k}'}(\mathbf{q}, \omega). \end{aligned} \quad (1.84)$$

Since

$$\begin{aligned} \int \frac{d\Omega}{4\pi} P_l(\theta) &= \delta_{l0}, \\ \int \frac{d\Omega}{4\pi} \delta(q v_F \cos \theta) &= \frac{1}{2 q v_F} \end{aligned}$$

it follows from Eq. (1.83) that

$$\int \frac{d\Omega_{\mathbf{k}}}{4\pi} \frac{d\Omega_{\mathbf{k}'}}{4\pi} \delta A_{\mathbf{k}\mathbf{k}'}(\mathbf{q}, \omega) + F_0 \int \frac{d\Omega_{\mathbf{p}}}{4\pi} \frac{d\Omega_{\mathbf{k}'}}{4\pi} \delta A_{\mathbf{p}\mathbf{k}'}(\mathbf{q}, \omega) = -\pi i \omega \frac{1}{V\mathcal{N}} \frac{1}{2 q v_F} F_0 A_0,$$

namely

$$\int \frac{d\Omega_{\mathbf{k}}}{4\pi} \frac{d\Omega_{\mathbf{k}'}}{4\pi} \delta A_{\mathbf{k}\mathbf{k}'}(\mathbf{q}, \omega) = -\pi i \omega \frac{1}{V\mathcal{N}} \frac{1}{2 q v_F} \frac{F_0}{1 + F_0} A_0 = -\pi i \omega \frac{1}{V\mathcal{N}} \frac{1}{2 q v_F} A_0^2.$$

Therefore Eq. (1.84) is found to be

$$\begin{aligned}
\chi(\mathbf{q}, \omega) &\simeq -\mathcal{N} (1 - A_0) \\
&\quad - i \pi \frac{\omega}{2 q v_F} \mathcal{N} (1 - A_0) \\
&\quad + i \pi \frac{\omega}{2 q v_F} \mathcal{N} A_0 \\
&\quad - i \pi \frac{\omega}{2 q v_F} \mathcal{N} A_0^2 \\
&= -\frac{\mathcal{N}}{1 + F_0} - i \pi \frac{\omega}{2 q v_F} \mathcal{N} (1 - A_0)^2 \\
&= -\frac{\mathcal{N}}{1 + F_0} - i \pi \frac{\omega}{2 q v_F} \mathcal{N} (1 + F_0)^{-2}.
\end{aligned} \tag{1.85}$$

1.6.3 High frequency limit of the response functions

Let us now consider the case $\omega \gg v_F q \rightarrow 0$ when (again the S and A indices are not explicitly shown)

$$A_{\mathbf{p}\mathbf{k}'}(\mathbf{q}, \omega) = f_{\mathbf{k}\mathbf{k}'}.$$

In this case

$$\frac{\mathbf{q} \cdot \mathbf{v}_k}{\mathbf{q} \cdot \mathbf{v}_k - \omega} \simeq -\frac{\mathbf{q} \cdot \mathbf{v}_k}{\omega} - \frac{(\mathbf{q} \cdot \mathbf{v}_k)^2}{\omega^2},$$

and, since the angular average of $\mathbf{q} \cdot \mathbf{v}_k$ vanishes, the response functions are

$$\begin{aligned}
\chi(\mathbf{q} \rightarrow \mathbf{0}, \omega) &= -\frac{2}{\omega^2 V} \sum_{\mathbf{k}} \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} (\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}})^2 \\
&\quad + \frac{4}{\omega^2 V} \sum_{\mathbf{k}\mathbf{k}'} (\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}}) (\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}'}) \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \frac{\partial n_{\mathbf{k}'}^0}{\partial \epsilon_{\mathbf{k}'}} f_{\mathbf{k}\mathbf{k}'}.
\end{aligned} \tag{1.86}$$

We note that

$$\begin{aligned}
\frac{2}{V} \sum_{\mathbf{k}} \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} (\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}})^2 &= -\mathcal{N} \int \frac{d\Omega}{4\pi} (v_F q \cos \theta)^2 \\
&= -\frac{1}{3} \mathcal{N} v_F^2 q^2, \\
\frac{4}{V} \sum_{\mathbf{k}\mathbf{k}'} \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \frac{\partial n_{\mathbf{k}'}^0}{\partial \epsilon_{\mathbf{k}'}} f_{\mathbf{k}\mathbf{k}'} (\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}}) (\mathbf{q} \cdot \mathbf{v}_{\mathbf{k}'}) &= \mathcal{N} v_F^2 q^2 \\
&\quad \times \sum_l F_l \int \frac{d\Omega_{\mathbf{k}}}{4\pi} \frac{d\Omega_{\mathbf{k}'}}{4\pi} \cos \theta_{\mathbf{k}} \cos \theta_{\mathbf{k}'} P_l(\theta_{\mathbf{k}\mathbf{k}'})
\end{aligned}$$

$$\begin{aligned}
&= \mathcal{N} v_F^2 q^2, \sum_{lm} F_l \int \frac{d\Omega_{\mathbf{k}}}{4\pi} \frac{d\Omega_{\mathbf{k}'}}{4\pi} \\
&\quad \times \sqrt{\frac{4\pi}{3}} Y_{10}(\theta_{\mathbf{k}}) \sqrt{\frac{4\pi}{3}} Y_{10}(\theta_{\mathbf{k}'}) \frac{4\pi}{2l+1} Y_{lm}^*(\theta_{\mathbf{k}}) Y_{lm}(\theta_{\mathbf{k}'}) \\
&= \mathcal{N} v_F^2 q^2 F_1 \frac{1}{9}.
\end{aligned}$$

Therefore Eq. (1.86) is

$$\chi(\mathbf{q} \rightarrow \mathbf{0}, \omega) = \mathcal{N} \frac{v_F^2 q^2}{3\omega^2} \left(1 + \frac{F_1}{3}\right). \quad (1.87)$$

In a system that is also translationally invariant, besides being isotropic, in the *S* channel the following relations hold

$$\begin{aligned}
\mathcal{N} &= \frac{m_* k_F}{\pi^2} = \frac{m k_F}{\pi^2} \left(1 + \frac{F_1}{3}\right), \\
v_F &= \frac{k_F}{m_*} = \frac{k_F}{m} \left(1 + \frac{F_1}{3}\right)^{-1}, \\
n &= \frac{k_F^3}{3\pi^2},
\end{aligned}$$

hence

$$\kappa(\mathbf{q} \rightarrow \mathbf{0}, \omega) = \frac{n}{m} \frac{q^2}{\omega^2}, \quad (1.88)$$

in agreement with the *f*-sum rule.

1.7 Charged Fermi-liquids: the Landau-Silin theory

Now, instead of a neutral Fermi system, let us consider a charged one and discuss how all previous results change. The first thing to note is that the quasiparticle interaction $f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}(\mathbf{x} - \mathbf{y})$ in Eq. (1.33) will now contain, besides a short range contribution, also a long range Coulomb one, so that can be assumed to be of the form

$$f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}(\mathbf{x} - \mathbf{y}) = f_{\mathbf{k}\sigma\mathbf{k}'\sigma'} \delta(\mathbf{x} - \mathbf{y}) + \frac{e^2}{|\mathbf{x} - \mathbf{y}|}. \quad (1.89)$$

Another novel feature that we have to take into account is the possible presence of a transverse electromagnetic field. If the system is translationally invariant or if inter-band matrix elements of the current density are negligible, the role of a transverse field is that the conjugate momentum is not anymore \mathbf{k} but

$$\mathbf{K} = \mathbf{k} - \frac{e}{c} \mathbf{A}(\mathbf{x}, t),$$

where \mathbf{A} is the transverse vector potential felt by the real electrons. Thus the quasiparticle occupation density in the semi-classical limit can be still parametrized by $n_{\mathbf{K}\sigma}(\mathbf{x}, t)$. Therefore

$$\begin{aligned} \left(\frac{\partial n_{\mathbf{K}\sigma}(\mathbf{x}, t)}{\partial t} \right)_{\mathbf{K}\mathbf{x}} &= \left(\frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial t} \right)_{\mathbf{k}\mathbf{x}} + \frac{e}{c} \frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{k}} \cdot \frac{\partial \mathbf{A}(\mathbf{x}, t)}{\partial t}, \\ \left(\frac{\partial n_{\mathbf{K}\sigma}(\mathbf{x}, t)}{\partial \mathbf{x}} \right)_{\mathbf{K}} &= \left(\frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{x}} \right)_{\mathbf{k}} + \sum_i \frac{e}{c} \frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial k_i} \frac{\partial A_i(\mathbf{x}, t)}{\partial \mathbf{x}}, \\ \left(\frac{\partial n_{\mathbf{K}\sigma}(\mathbf{x}, t)}{\partial \mathbf{K}} \right)_{\mathbf{x}} &= \left(\frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{k}} \right)_{\mathbf{x}}. \end{aligned}$$

We also note that, in the presence of \mathbf{A} the quasiparticle excitation energy, Eq. (1.34), changes into

$$\bar{\epsilon}_{\mathbf{k}\sigma}(\mathbf{x}, t) \rightarrow \bar{\epsilon}_{\mathbf{K}+e\mathbf{A}/c\sigma}(\mathbf{x}, t) = \bar{\epsilon}_{\mathbf{k}\sigma}(\mathbf{x}, t),$$

so that

$$\frac{\partial \bar{\epsilon}_{\mathbf{K}+e\mathbf{A}/c\sigma}(\mathbf{x}, t)}{\partial \mathbf{K}} = \frac{\partial \bar{\epsilon}_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{k}} = \mathbf{v}_{\mathbf{k}\sigma}(\mathbf{x}, t),$$

is the proper quasiparticle group velocity. On the other hand

$$\begin{aligned} \frac{\partial \bar{\epsilon}_{\mathbf{K}+e\mathbf{A}/c\sigma}(\mathbf{x}, t)}{\partial \mathbf{x}} &= \sum_i \frac{e}{c} v_{\mathbf{k}\sigma i}(\mathbf{x}, t) \frac{\partial A_i(\mathbf{x}, t)}{\partial \mathbf{x}} \\ &\quad + \frac{\partial V_\sigma(\mathbf{x}, t)}{\partial \mathbf{x}} + \sum_{\mathbf{k}'\sigma'} \int d\mathbf{y} f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}(\mathbf{x} - \mathbf{y}) \frac{\partial n_{\mathbf{k}'\sigma'}(\mathbf{y}, t)}{\partial \mathbf{y}}. \end{aligned}$$

Putting everything together we find the following transport equation for charged electrons:

$$\begin{aligned}
I_{\mathbf{k}\sigma}(\mathbf{x}, t) = & \frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial t} + \frac{e}{c} \frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{k}} \cdot \frac{\partial \mathbf{A}(\mathbf{x}, t)}{\partial t} \\
& + \mathbf{v}_{\mathbf{k}\sigma}(\mathbf{x}, t) \cdot \frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{x}} + \sum_{ij} v_{\mathbf{k}\sigma j}(\mathbf{x}, t) \frac{e}{c} \frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial k_i} \frac{\partial A_i(\mathbf{x}, t)}{\partial x_j} \\
& - \frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{k}} \cdot \left[\frac{\partial V_\sigma(\mathbf{x}, t)}{\partial \mathbf{x}} + \sum_{\mathbf{k}'\sigma'} \int d\mathbf{y} f_{\mathbf{k}\sigma \mathbf{k}'\sigma'}(\mathbf{x} - \mathbf{y}) \frac{\partial n_{\mathbf{k}'\sigma'}(\mathbf{y}, t)}{\partial \mathbf{y}} \right] \\
& - \sum_{ij} \frac{e}{c} \frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial k_j} v_{\mathbf{k}\sigma i}(\mathbf{x}, t) \frac{\partial A_i(\mathbf{x}, t)}{\partial x_j}
\end{aligned}$$

We note that the two terms with the \sum_{ij} can be written as

$$\begin{aligned}
& \sum_{ij} \frac{e}{c} \frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial k_i} v_{\mathbf{k}\sigma j}(\mathbf{x}, t) \left(\frac{\partial A_i(\mathbf{x}, t)}{\partial x_j} - \frac{\partial A_j(\mathbf{x}, t)}{\partial x_i} \right) \\
& = -\frac{e}{c} (\mathbf{v}_{\mathbf{k}\sigma}(\mathbf{x}, t) \times \mathbf{H}(\mathbf{x}, t)) \cdot \frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{k}},
\end{aligned}$$

where

$$\mathbf{H}(\mathbf{x}, t) = \nabla \times \mathbf{A}(\mathbf{x}, t)$$

is the magnetic field. Since the external transverse electric field is

$$\mathbf{E}(\mathbf{x}, t) = -\frac{1}{c} \frac{\partial \mathbf{A}(\mathbf{x}, t)}{\partial t},$$

the final expression of the transport equation reads

$$\begin{aligned}
I_{\mathbf{k}\sigma}(\mathbf{x}, t) = & \frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial t} + \mathbf{v}_{\mathbf{k}\sigma}(\mathbf{x}, t) \cdot \frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{x}} \\
& - \frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{k}} \cdot \left[\frac{\partial V_\sigma(\mathbf{x}, t)}{\partial \mathbf{x}} + \sum_{\mathbf{k}'\sigma'} \int d\mathbf{y} f_{\mathbf{k}\sigma \mathbf{k}'\sigma'}(\mathbf{x} - \mathbf{y}) \frac{\partial n_{\mathbf{k}'\sigma'}(\mathbf{y}, t)}{\partial \mathbf{y}} \right] \\
& - e \frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{k}} \cdot \mathbf{E}(\mathbf{x}, t) - \frac{e}{c} (\mathbf{v}_{\mathbf{k}\sigma}(\mathbf{x}, t) \times \mathbf{H}(\mathbf{x}, t)) \cdot \frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{k}}. \quad (1.90)
\end{aligned}$$

Let us now expand the transport equation (1.90) at linear order in the deviation from equilibrium

$$n_{\mathbf{k}\sigma}(\mathbf{x}, t) = n_{\mathbf{k}\sigma}^0 + \delta n_{\mathbf{k}\sigma}(\mathbf{x}, t).$$

First we assume an ac electromagnetic field acting as a perturbation, in which case

$$-\frac{e}{c} (\mathbf{v}_{\mathbf{k}\sigma}(\mathbf{x}, t) \times \mathbf{H}(\mathbf{x}, t)) \cdot \frac{\partial n_{\mathbf{k}\sigma}(\mathbf{x}, t)}{\partial \mathbf{k}} \simeq -\frac{e}{c} (\mathbf{v}_{\mathbf{k}} \times \mathbf{H}(\mathbf{x}, t)) \cdot \frac{\partial n_{\mathbf{k}}^0}{\partial \mathbf{k}}$$

$$= -\frac{e}{c} \left(\mathbf{v}_k \times \mathbf{H}(\mathbf{x}, t) \right) \cdot \frac{\partial n_k^0}{\partial \epsilon_k} \mathbf{v}_k = 0.$$

This shows that an ac magnetic field does not contribute to the linearized transport equation, that becomes

$$\begin{aligned} I_{k\sigma}(\mathbf{x}, t) &= \frac{\partial \delta n_{k\sigma}(\mathbf{x}, t)}{\partial t} + \mathbf{v}_k \cdot \frac{\partial \delta n_{k\sigma}(\mathbf{x}, t)}{\partial \mathbf{x}} \\ &\quad + \frac{\partial n_k^0}{\partial \epsilon_k} \mathbf{v}_k \cdot \left[-\frac{\partial V_\sigma(\mathbf{x}, t)}{\partial \mathbf{x}} - e \mathbf{E}(\mathbf{x}, t) - \sum_{\mathbf{k}'\sigma'} \int d\mathbf{y} f_{k\sigma k'\sigma'}(\mathbf{x} - \mathbf{y}) \frac{\partial \delta n_{k'\sigma'}(\mathbf{y}, t)}{\partial \mathbf{y}} \right] \\ &= \frac{\partial \delta n_{k\sigma}(\mathbf{x}, t)}{\partial t} + \mathbf{v}_k \cdot \frac{\partial \delta \bar{n}_{k\sigma}(\mathbf{x}, t)}{\partial \mathbf{x}} \\ &\quad + \frac{\partial n_k^0}{\partial \epsilon_k} \mathbf{v}_k \cdot \left[-\frac{\partial V_\sigma(\mathbf{x}, t)}{\partial \mathbf{x}} - e \mathbf{E}(\mathbf{x}, t) \right], \end{aligned} \quad (1.91)$$

where we recall that

$$\delta \bar{n}_{k\sigma}(\mathbf{x}, t) = \delta n_{k\sigma}(\mathbf{x}, t) - \frac{\partial n_k^0}{\partial \epsilon_k} \sum_{\mathbf{k}'\sigma'} \int d\mathbf{y} f_{k\sigma k'\sigma'}(\mathbf{x} - \mathbf{y}) \delta n_{k'\sigma'}(\mathbf{y}, t),$$

is the deviation from local equilibrium.

In the presence of a dc magnetic field $\mathbf{H}(\mathbf{x})$, a subtle issue arises in connection with the Lorenz's force term

$$-\frac{e}{c} \left(\mathbf{v}_{k\sigma}(\mathbf{x}, t) \times \mathbf{H}(\mathbf{x}, t) \right) \cdot \frac{\partial n_{k\sigma}(\mathbf{x}, t)}{\partial \mathbf{k}}.$$

Indeed, a dc field, unlike an ac one, can be assumed as integral part of the unperturbed Hamiltonian and, if large, can be taken as a zeroth order term, $\mathbf{H}(\mathbf{x}) = \mathbf{H}_0(\mathbf{x})$. This requires to expand at linear order $\mathbf{v}_{k\sigma}(\mathbf{x}, t)$ and $\partial n_{k\sigma}(\mathbf{x}, t)/\partial \mathbf{k}$,

$$\begin{aligned} \mathbf{v}_{k\sigma}(\mathbf{x}, t) &\simeq \mathbf{v}_{k\sigma} + \sum_{\mathbf{k}'\sigma'} \int d\mathbf{y} \frac{\partial}{\partial \mathbf{k}} \left[f_{k\sigma k'\sigma'}(\mathbf{x} - \mathbf{y}) \frac{\partial \delta n_{k'\sigma'}(\mathbf{y}, t)}{\partial \mathbf{y}} \right], \\ \frac{\partial n_{k\sigma}(\mathbf{x}, t)}{\partial \mathbf{k}} &\simeq \frac{\partial n_k^0}{\partial \mathbf{k}} + \frac{\partial \delta n_{k\sigma}(\mathbf{x}, t)}{\partial \mathbf{k}}, \end{aligned}$$

leading to the transport equation

$$\begin{aligned} I_{k\sigma}(\mathbf{x}, t) &= \frac{\partial \delta n_{k\sigma}(\mathbf{x}, t)}{\partial t} + \mathbf{v}_k \cdot \frac{\partial \delta \bar{n}_{k\sigma}(\mathbf{x}, t)}{\partial \mathbf{x}} \\ &\quad + \frac{\partial n_k^0}{\partial \epsilon_k} \mathbf{v}_k \cdot \left[-\frac{\partial V_\sigma(\mathbf{x}, t)}{\partial \mathbf{x}} - e \mathbf{E}(\mathbf{x}, t) \right] - \frac{e}{c} \left(\mathbf{v}_k \times \mathbf{H}_0(\mathbf{x}, t) \right) \cdot \frac{\partial \delta \bar{n}_{k\sigma}(\mathbf{x}, t)}{\partial \mathbf{k}} \end{aligned} \quad (1.92)$$

which is the appropriate one to discuss properties like magnetoresistance, cyclotron resonances, etc. However, in what follows we will not consider such a physical situation of a large dc field, hence we will just focus on Eq. (1.91).

1.7.1 Formal solution of the transport equation

We note that, because of (1.89),

$$f_{\mathbf{kk}'}^S(\mathbf{x} - \mathbf{y}) = f_{\mathbf{kk}'}^S \delta(\mathbf{x} - \mathbf{y}) + \frac{e^2}{|\mathbf{x} - \mathbf{y}|}, \quad f_{\mathbf{kk}'}^A(\mathbf{x} - \mathbf{y}) = f_{\mathbf{kk}'}^A \delta(\mathbf{x} - \mathbf{y}), \quad (1.93)$$

showing that only the response in the S charge-channel is going to be modified by the Coulomb repulsion with respect to the previously studied case of neutral particles. Hence let us assume that

$$V_\sigma(\mathbf{x}, t) = -e \phi(\mathbf{x}, t),$$

is the conventional scalar potential and, neglecting the collision integral, let us write the transport equation for the charge deviation

$$\delta n_{\mathbf{k}}(\mathbf{x}, t) = \delta n_{\mathbf{k}\uparrow}(\mathbf{x}, t) + \delta n_{\mathbf{k}\downarrow}(\mathbf{x}, t),$$

which is found to be

$$\frac{\partial \delta n_{\mathbf{k}}(\mathbf{x}, t)}{\partial t} + \mathbf{v}_{\mathbf{k}} \cdot \frac{\partial \delta \bar{n}_{\mathbf{k}}(\mathbf{x}, t)}{\partial \mathbf{x}} - 2 \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \mathbf{v}_{\mathbf{k}} \cdot \left[-e \frac{\partial \phi(\mathbf{x}, t)}{\partial \mathbf{x}} - e \mathbf{E}(\mathbf{x}, t) \right] = 0, \quad (1.94)$$

with

$$\delta \bar{n}_{\mathbf{k}}(\mathbf{x}, t) = \delta n_{\mathbf{k}}(\mathbf{x}, t) - 2 \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \sum_{\mathbf{k}'} \int d\mathbf{y} f_{\mathbf{kk}'}^S(\mathbf{x} - \mathbf{y}) \delta n_{\mathbf{k}'}(\mathbf{y}, t).$$

In the Fourier space

$$\delta \bar{n}_{\mathbf{k}}(\mathbf{q}, \omega) = \delta n_{\mathbf{k}}(\mathbf{q}, \omega) - 2 \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \sum_{\mathbf{k}'} f_{\mathbf{kk}'}^S \delta n_{\mathbf{k}'}(\mathbf{q}, \omega) - 2 \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \frac{4\pi e^2}{q^2} \delta \rho(\mathbf{q}, \omega),$$

where

$$\delta \rho(\mathbf{q}, \omega) = \frac{1}{V} \sum_{\mathbf{k}'} \delta n_{\mathbf{k}'}(\mathbf{q}, \omega),$$

is the deviation of the total charge density. We then find

$$\begin{aligned} & (\omega - \mathbf{v}_{\mathbf{k}} \cdot \mathbf{q}) \delta n_{\mathbf{k}}(\mathbf{q}, \omega) + 2 \mathbf{v}_{\mathbf{k}} \cdot \mathbf{q} \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \sum_{\mathbf{k}'} f_{\mathbf{kk}'}^S \delta n_{\mathbf{k}'}(\mathbf{q}, \omega) \\ & - i e 2 \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \mathbf{v}_{\mathbf{k}} \cdot \mathcal{E}(\mathbf{q}, \omega) = 0, \end{aligned} \quad (1.95)$$

where $\mathcal{E}(\mathbf{q}, \omega)$ is the internal electric field felt by the quasiparticles,

$$\mathcal{E}(\mathbf{q}, \omega) = \mathbf{E}(\mathbf{q}, \omega) - i \mathbf{q} \phi(\mathbf{q}, \omega) + i 4 \pi e \frac{\mathbf{q}}{q^2} \delta \rho(\mathbf{q}, \omega), \quad (1.96)$$

that contains the external transverse and longitudinal fields as well as the longitudinal field created by the same quasiparticles.

Longitudinal response

Let us assume a zero transverse field, and define as

$$V(\mathbf{q}, \omega) = -e\phi(\mathbf{q}, \omega) + \frac{4\pi e^2}{q^2} \delta\rho(\mathbf{q}, \omega), \quad (1.97)$$

the internal scalar potential. One easily recognizes that the response to the internal scalar potential is formally the same as for neutral particles, so that, by means of Eq. (1.79), we find that

$$\delta\rho(\mathbf{q}, \omega) = \chi^S(\mathbf{q}, \omega) V(\mathbf{q}, \omega) \equiv \chi_*(\mathbf{q}, \omega) V(\mathbf{q}, \omega), \quad (1.98)$$

that also define the so-called “proper” charge response-function χ_* . Inserting the expression of $V(\mathbf{q}, \omega)$, Eq. (1.97), and solving for $\delta\rho(\mathbf{q}, \omega)$ we finally obtain

$$\delta\rho(\mathbf{q}, \omega) = \frac{\chi_*(\mathbf{q}, \omega)}{1 - \frac{4\pi e^2}{q^2} \chi_*(\mathbf{q}, \omega)} V(\mathbf{q}, \omega) \equiv \chi(\mathbf{q}, \omega) V(\mathbf{q}, \omega),, \quad (1.99)$$

that defines the “improper” response function χ , which is the response to the external field, as opposed to the proper one, i.e. the response to the internal field.

Eq.(1.99) provides the definition of the longitudinal dielectric constant $\epsilon_{||}(\mathbf{q}, \omega)$ as

$$\epsilon_{||}(\mathbf{q}, \omega) = 1 - \frac{4\pi e^2}{q^2} \chi_*(\mathbf{q}, \omega). \quad (1.100)$$

In the limit $\omega \rightarrow 0$ first and then $q \rightarrow 0$, we can make use of Eq. (1.85) and find that

$$\lim_{q \rightarrow 0} \lim_{\omega \rightarrow 0} \epsilon_{||}(\mathbf{q}, \omega) = \lim_{q \rightarrow 0} 1 + \frac{4\pi e^2}{q^2} \frac{\mathcal{N}}{1 + F_0^S} \rightarrow \infty, \quad (1.101)$$

which defines the effective Thomas-Fermi screening-length

$$\lambda_{TF} = \sqrt{\frac{\pi(1 + F_0^S)}{e^2 \mathcal{N}}}.$$

In the limit $q \rightarrow 0$, we can use Eq. (1.87) to get

$$\lim_{q \rightarrow 0} \epsilon_{||}(\mathbf{q}, \omega) = 1 - \frac{4\pi e^2}{q^2} \mathcal{N} \frac{v_F^2 q^2}{3\omega^2} \left(1 + \frac{F_1}{3}\right) \equiv 1 - \frac{\omega_p^2}{\omega^2}, \quad (1.102)$$

that provides the definition of the conduction-band plasma-frequency

$$\omega_p^2 = \frac{4\pi e^2 \mathcal{N} v_F^2}{3} \left(1 + \frac{F_1}{3}\right), \quad (1.103)$$

as the pole of $1/\epsilon_{||}(\mathbf{0}, \omega)$. Note that, for a translationally invariant system

$$\omega_p^2 = \frac{4\pi n e^2}{m},$$

with n the electron density and m the real electron mass, that coincides with the conventional expression for the plasma oscillations.

1.8 Dirty quasiparticle gas

So far we have not taken into account the collision integral, that is however important at frequencies smaller than the typical collision rate. At very low temperature T , the main contribution to the collision rate comes from impurity scattering. Indeed, collisions due to phonons vanish at low temperature, as phonon occupations go exponentially to zero as $T \rightarrow 0$, as well as collisions due to scattering off other quasiparticles.⁶ Taking into account only the scattering off (non-magnetic) impurities, and moreover assuming a short-range impurity potential, we can write the collision integral as

$$I_{\mathbf{k}\sigma}(\mathbf{x}, t) = -2\pi \sum_{\mathbf{p}} W_{\mathbf{k}\mathbf{p}} \left[n_{\mathbf{k}\sigma}(\mathbf{x}, t) (1 - n_{\mathbf{p}\sigma}(\mathbf{x}, t)) - n_{\mathbf{p}\sigma}(\mathbf{x}, t) (1 - n_{\mathbf{k}\sigma}(\mathbf{x}, t)) \right] \times \delta(\bar{\epsilon}_{\mathbf{k}\sigma}(\mathbf{x}, t) - \bar{\epsilon}_{\mathbf{p}\sigma}(\mathbf{x}, t)), \quad (1.104)$$

⁶An excited quasiparticle at $\bar{\epsilon}_{\mathbf{k}} > \mu$ can in principle decay into a quasiparticle at momentum \mathbf{k}' with $\bar{\epsilon}_{\mathbf{k}'} > \mu$ plus a quasiparticle-quasihole pair, namely a quasiparticle with momentum \mathbf{p}' with $\bar{\epsilon}_{\mathbf{p}'} > \mu$ and a quasihole with momentum \mathbf{p} and energy $\bar{\epsilon}_{\mathbf{p}} < \mu$. Because of momentum conservation $\mathbf{k} = \mathbf{k}' + \mathbf{p}' - \mathbf{p}$, and of energy conservation

$$\bar{\epsilon}_{\mathbf{k}} - \mu = (\bar{\epsilon}_{\mathbf{k}'} - \mu) + (\bar{\epsilon}_{\mathbf{p}'} - \mu) - (\bar{\epsilon}_{\mathbf{p}} - \mu).$$

The collision integral expressed through the Fermi golden-rule will have the general form (we discard for simplicity the spin label)

$$I_{\mathbf{k}} = \frac{1}{V^2} \sum_{\mathbf{k}' \mathbf{p} \mathbf{p}'} W_{\mathbf{k}\mathbf{p} \mathbf{p}' \mathbf{k}'} \delta(\mathbf{k} + \mathbf{p} - \mathbf{k}' - \mathbf{p}') \delta(\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{p}} - \epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{p}'}) n_{\mathbf{k}} n_{\mathbf{k}'} n_{\mathbf{p}'} (1 - n_{\mathbf{p}}),$$

where W is the modulus square of the scattering amplitude. Since one momentum is fixed by the momentum conservation, say \mathbf{p} , the sum becomes a double sum over \mathbf{k}' and \mathbf{p}' with the condition that

$$|\bar{\epsilon}_{\mathbf{k}'} - \mu| + |\bar{\epsilon}_{\mathbf{p}'} - \mu| + |\bar{\epsilon}_{\mathbf{k}'+\mathbf{p}'-\mathbf{k}} - \mu| = |\bar{\epsilon}_{\mathbf{k}'} - \mu| \simeq T,$$

the last almost equivalence deriving from the fact that the energy variation with respect to the chemical potential of a quasiparticle excitation at temperature T is of the order of T itself. This implies that both $(\bar{\epsilon}_{\mathbf{k}'} - \mu)$ and $(\bar{\epsilon}_{\mathbf{p}'} - \mu)$ are positive but smaller than T , so that, by simple phase space arguments, the collision integral is found to decay approximately as T^2 . Extending this analysis, one readily realizes that any decay into a quasiparticle plus m quasiparticle-quasihole pairs occurs with probability T^{2m} . Therefore the collision integral due to scattering off quasiparticles is negligible at low temperatures.

where the energy conservation involves, as it should, the true quasiparticle excitation energy

$$\bar{\epsilon}_{\mathbf{k}\sigma}(\mathbf{x}, t) = \frac{\delta E}{\delta n_{\mathbf{k}\sigma}(\mathbf{x}, t)} = \epsilon_{\mathbf{k}} + \sum_{\mathbf{k}'\sigma'} \int d\mathbf{y} f_{\mathbf{k}\sigma\mathbf{k}'\sigma'}(\mathbf{x} - \mathbf{y}) \delta n_{\mathbf{k}'\sigma'}(\mathbf{y}, t).$$

We note that

$$\begin{aligned} & \left[n_{\mathbf{k}\sigma}(\mathbf{x}, t) (1 - n_{\mathbf{p}\sigma}(\mathbf{x}, t)) - n_{\mathbf{p}\sigma}(\mathbf{x}, t) (1 - n_{\mathbf{k}\sigma}(\mathbf{x}, t)) \right] \delta(\bar{\epsilon}_{\mathbf{k}\sigma}(\mathbf{x}, t) - \bar{\epsilon}_{\mathbf{p}\sigma}(\mathbf{x}, t)) \\ &= \left[n_{\mathbf{k}\sigma}(\mathbf{x}, t) - n_{\mathbf{p}\sigma}(\mathbf{x}, t) \right] \delta(\bar{\epsilon}_{\mathbf{k}\sigma}(\mathbf{x}, t) - \bar{\epsilon}_{\mathbf{p}\sigma}(\mathbf{x}, t)) \\ &= \left[\bar{n}_{\mathbf{k}\sigma}^0(\mathbf{x}, t) - \bar{n}_{\mathbf{p}\sigma}^0(\mathbf{x}, t) + \delta\bar{n}_{\mathbf{k}\sigma}(\mathbf{x}, t) - \delta\bar{n}_{\mathbf{p}\sigma}(\mathbf{x}, t) \right] \delta(\bar{\epsilon}_{\mathbf{k}\sigma}(\mathbf{x}, t) - \bar{\epsilon}_{\mathbf{p}\sigma}(\mathbf{x}, t)) \\ &= \left[\delta\bar{n}_{\mathbf{k}\sigma}(\mathbf{x}, t) - \delta\bar{n}_{\mathbf{p}\sigma}(\mathbf{x}, t) \right] \delta(\bar{\epsilon}_{\mathbf{k}\sigma}(\mathbf{x}, t) - \bar{\epsilon}_{\mathbf{p}\sigma}(\mathbf{x}, t)), \end{aligned}$$

so that

$$I_{\mathbf{k}\sigma}(\mathbf{x}, t) = -2\pi \sum_{\mathbf{p}} W_{\mathbf{k}\mathbf{p}} \left[\delta\bar{n}_{\mathbf{k}\sigma}(\mathbf{x}, t) - \delta\bar{n}_{\mathbf{p}\sigma}(\mathbf{x}, t) \right] \delta(\bar{\epsilon}_{\mathbf{k}\sigma}(\mathbf{x}, t) - \bar{\epsilon}_{\mathbf{p}\sigma}(\mathbf{x}, t)), \quad (1.105)$$

showing that the collision integral only depends upon deviations from local equilibrium. Within linear approximation

$$I_{\mathbf{k}\sigma}(\mathbf{x}, t) \simeq -2\pi \sum_{\mathbf{p}} W_{\mathbf{k}\mathbf{p}} \left[\delta\bar{n}_{\mathbf{k}\sigma}(\mathbf{x}, t) - \delta\bar{n}_{\mathbf{p}\sigma}(\mathbf{x}, t) \right] \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{p}}). \quad (1.106)$$

Let us write

$$\begin{aligned} W_{\mathbf{k}\mathbf{p}} &= \frac{1}{V} \sum_l W_l P_l(\theta_{\mathbf{k}\mathbf{p}}), \\ \delta\bar{n}_{\mathbf{k}\sigma}(\mathbf{x}, t) &= -\frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \sum_{lm} \delta\bar{n}_{lm\sigma}(\mathbf{x}, t) Y_{lm}(\Omega_{\mathbf{k}}) \end{aligned}$$

so that Eq. (1.106) becomes

$$\begin{aligned} I_{\mathbf{k}\sigma}(\mathbf{x}, t) &= \pi \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \mathcal{N} \sum_{lm} W_0 \delta\bar{n}_{lm\sigma}(\mathbf{x}, t) Y_{lm}(\Omega_{\mathbf{k}}) \\ &\quad - \pi \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \mathcal{N} \sum_{lm} \frac{W_l}{2l+1} \delta\bar{n}_{lm\sigma}(\mathbf{x}, t) Y_{lm}(\Omega_{\mathbf{k}}) \\ &= \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \sum_{lm} \frac{1}{\tau_l} \delta\bar{n}_{lm\sigma}(\mathbf{x}, t) Y_{lm}(\Omega_{\mathbf{k}}), \end{aligned} \quad (1.107)$$

where the inverse relaxation time is defined through

$$\begin{aligned}\frac{1}{\tau_l} &= \pi \mathcal{N} \left(W_0 - \frac{W_l}{2l+1} \right) \\ &= \frac{2\pi}{V} \sum_{\mathbf{p}} W_{\mathbf{kp}} \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{p}}) \left[1 - P_l(\theta_{\mathbf{kp}}) \right].\end{aligned}\quad (1.108)$$

We note that $1/\tau_0 = 0$.

Therefore the transport equation in Fourier space and for the charge S component reads

$$\begin{aligned}-\omega \delta n_{\mathbf{k}}(\mathbf{q}, \omega) + \mathbf{q} \cdot \mathbf{v}_{\mathbf{k}} \delta n_{\mathbf{k}}(\mathbf{q}, \omega) - 2 \frac{\partial n_{\mathbf{k}}^0}{\partial \mathbf{k}} \mathbf{q} \cdot \mathbf{v}_{\mathbf{k}} \sum_{\mathbf{k}'} f_{\mathbf{kk}'}^S \delta n_{\mathbf{k}'}(\mathbf{q}, \omega) \\ + i e 2 \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \mathbf{v}_{\mathbf{k}} \cdot \boldsymbol{\mathcal{E}}(\mathbf{q}, \omega) = -i \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \sum_{lm} \frac{1}{\tau_l} \delta \bar{n}_{lm}(\mathbf{q}, \omega) Y_{lm}(\Omega_{\mathbf{k}}) \\ = -\omega \delta n_{\mathbf{k}}(\mathbf{q}, \omega) + \mathbf{q} \cdot \mathbf{v}_{\mathbf{k}} \delta \bar{n}_{\mathbf{k}}(\mathbf{q}, \omega) + i e 2 \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \mathbf{v}_{\mathbf{k}} \cdot \boldsymbol{\mathcal{E}}(\mathbf{q}, \omega),\end{aligned}\quad (1.109)$$

where we recall that

$$\boldsymbol{\mathcal{E}}(\mathbf{q}, \omega) = \mathbf{E}(\mathbf{q}, \omega) + i 4\pi e \frac{\mathbf{q}}{q^2} \delta \rho(\mathbf{q}, \omega), \quad (1.110)$$

is the internal field felt by quasiparticles, \mathbf{E} including both transverse and longitudinal components, and we have defined

$$\delta \bar{n}_{\mathbf{k}}(\mathbf{q}, \omega) = \delta n_{\mathbf{k}}(\mathbf{q}, \omega) - 2 \frac{\partial n_{\mathbf{k}}^0}{\partial \mathbf{k}} \sum_{\mathbf{k}'} f_{\mathbf{kk}'}^S \delta n_{\mathbf{k}'}(\mathbf{q}, \omega),$$

as the deviation from local equilibrium excluding the long-range interaction.

1.8.1 Conductivity

We observe that

$$-e \delta \rho(\mathbf{q} = \mathbf{0}, \omega) = \int dt e^{i\omega t} \delta N(t),$$

is the frequency Fourier-transform of the change in the total electron charge. If we assume that the system is maintained neutral at any time by a compensating positive ionic charge-density, then the $\mathbf{q} = \mathbf{0}$ component of the field generated by the electrons must be canceled exactly by the ionic field. In other words, $\delta \rho(\mathbf{q}, \omega)$ must not include any $\mathbf{q} = \mathbf{0}$ component, i.e. $\delta \rho(\mathbf{0}, \omega) = 0$. Thus, taking $q = 0$ in (1.109) we find

$$-\omega \delta n_{\mathbf{k}}(\omega) + i e 2 \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \mathbf{v}_{\mathbf{k}} \cdot \mathbf{E}(\omega) = -i \frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \sum_{lm} \frac{1}{\tau_l} \delta \bar{n}_{lm}(\omega) Y_{lm}(\Omega_{\mathbf{k}}). \quad (1.111)$$

We observe that

$$\begin{aligned}\mathbf{v}_k \cdot \mathbf{E}(\omega) &= \frac{1}{m_*} \mathbf{k} \cdot \mathbf{E}(\omega) = \frac{k}{m_*} \sqrt{\frac{4\pi}{3}} \left[Y_{10}(\Omega_k) E_z(\omega) \right. \\ &\quad \left. + Y_{1+1}(\Omega_k) \frac{1}{2} (E_x(\omega) - iE_y(\omega)) + Y_{1-1}(\Omega_k) \frac{1}{2} (E_x(\omega) + iE_y(\omega)) \right],\end{aligned}$$

namely that only the $l = 1$ components are coupled to the electric field, so that the actual transport equation reads [dropping the label $(l,m)=(1,m)$]

$$-\omega \delta n_k(\omega) + i e 2 \frac{\partial n_k^0}{\partial \epsilon_k} \mathbf{v}_k \cdot \mathbf{E}(\omega) = i \frac{1}{\tau_1} \delta \bar{n}_k(\omega).$$

Since, for $l = 1$ deviations

$$\delta n = \frac{\delta \bar{n}}{1 + \frac{F_1^S}{3}},$$

we finally get

$$\delta \bar{n}_k(\omega) = 2e \frac{\partial n_k^0}{\partial \epsilon_k} \left(1 + \frac{F_1^S}{3} \right) \frac{1}{-i\omega + \frac{1}{\tau}} \mathbf{v}_k \cdot \mathbf{E}(\omega), \quad (1.112)$$

where

$$\tau = \frac{\tau_1}{1 + \frac{F_1^S}{3}}. \quad (1.113)$$

The electric current is therefore

$$\begin{aligned}\mathbf{J}(\omega) &= -\frac{e}{V} \sum_k \mathbf{v}_k \delta \bar{n}_k(\omega) \\ &= -\frac{e}{V} \sum_k \mathbf{v}_k 2e \frac{\partial n_k^0}{\partial \epsilon_k} \left(1 + \frac{F_1^S}{3} \right) \frac{1}{-i\omega + \frac{1}{\tau}} \mathbf{v}_k \cdot \mathbf{E}(\omega)\end{aligned} \quad (1.114)$$

$$= e^2 \mathcal{N} \frac{v_F^2}{3} \left(1 + \frac{F_1^S}{3} \right) \frac{1}{-i\omega + \frac{1}{\tau}} \mathbf{E}(\omega) \equiv \sigma(\omega) \mathbf{E}(\omega), \quad (1.115)$$

which defines the conductivity $\sigma(\omega)$. We note that

$$\mathcal{N} \frac{v_F^2}{3} = \frac{m_* k_F}{\pi^2} \frac{k_F^2}{3m_*^2} = \frac{n}{m_*},$$

with n the average electron density. Thus the conductivity is

$$\sigma(\omega) = \frac{n e^2}{m_*} \left(1 + \frac{F_1^S}{3}\right) \frac{1}{-i\omega + \frac{1}{\tau}}, \quad (1.116)$$

with a dc value

$$\sigma = \sigma(0) = \frac{n e^2 \tau}{m_*} \left(1 + \frac{F_1^S}{3}\right). \quad (1.117)$$

This expression shows that the effective mass that controls dc transport is not m_* but

$$\frac{m_*}{1 + \frac{F_1^S}{3}},$$

which, for a system that is translationally invariant before adding the impurities, is just the real-electron mass m .

1.8.2 Diffusive behavior

Let us now consider a finite q such that $v_F q \tau \ll 1$ as well as $\omega \tau \ll 1$, and assume a longitudinal electric field $\mathbf{E} \parallel \mathbf{q}$, \mathbf{q} taken to be along the z -axis. If we write

$$\delta \bar{n}_{\mathbf{k}}(\mathbf{q}, \omega) = -\frac{\partial n_{\mathbf{k}}^0}{\partial \epsilon_{\mathbf{k}}} \sum_{lm} \delta \bar{n}_{lm}(\mathbf{q}, \omega) Y_{lm}(\Omega_{\mathbf{k}}),$$

and analogously for $\delta n_{\mathbf{k}}$, we note that only the $m = 0$ component is coupled to the external field. If we substitute these expressions for δn and $\delta \bar{n}$ into Eq. (1.109), multiply both sides of this equation by $Y_{l0}^*(\Omega_{\mathbf{k}})$ and integrate over the solid angle, by means of

$$\int d\Omega Y_{l0}^*(\Omega) Y_{l1,0}(\Omega) Y_{l2,0}(\Omega) = \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2l+1)}} \left(C_{l_1 0 l_2 0}^{l 0}\right)^2,$$

where $C_{l_1 0 l_2 0}^{l 0}$ are Clebsch-Gordan coefficients, we find the following set of equations (we discard the label $m = 0$)

$$-\omega \delta n_l(\mathbf{q}, \omega) + q v_F \sum_{l'} \sqrt{\frac{2l'+1}{2l+1}} \left(C_{l' 0 1 0}^{l 0}\right)^2 \delta \bar{n}_{l'}(\mathbf{q}, \omega) - 2 i e v_F \sqrt{\frac{4\pi}{3}} \mathcal{E}(\mathbf{q}, \omega) \delta_{l1} = i \frac{\delta \bar{n}_l(\mathbf{q}, \omega)}{\tau_l}. \quad (1.118)$$

We observe that only $l = 1$ is directly coupled to the field, so that, for any $l > 1$, we find

$$\begin{aligned} & \left(-\frac{\tau_l \omega}{1 + \frac{F_l^S}{2l+1}} - i \right) \delta \bar{n}_l(\mathbf{q}, \omega) + \tau_l q v_F \sum_{l' \neq 1} \sqrt{\frac{2l'+1}{2l+1}} \left(C_{l'010}^{l0} \right)^2 \delta \bar{n}_{l'}(\mathbf{q}, \omega) \\ &= -\tau_l q v_F \sqrt{\frac{3}{2l+1}} \left(C_{1010}^{l0} \right)^2 \delta \bar{n}_1(\mathbf{q}, \omega). \end{aligned}$$

This implies that all deviations with $l > 1$ are driven by $q v_F \tau_l \delta \bar{n}_1 \ll \delta \bar{n}_1$, therefore are negligible. What remains are just the components with $l = 0, 1$, satisfying the coupled equations

$$\begin{aligned} -\frac{\omega}{1 + F_0^S} \delta \bar{n}_0(\mathbf{q}, \omega) + q v_F \sqrt{\frac{1}{3}} \delta \bar{n}_1(\mathbf{q}, \omega) &= 0, \\ -\frac{\omega}{1 + F_1^S} \delta \bar{n}_1(\mathbf{q}, \omega) + q v_F \sqrt{\frac{1}{3}} \delta \bar{n}_0(\mathbf{q}, \omega) - 2i e v_F \sqrt{\frac{4\pi}{3}} \mathcal{E}(\mathbf{q}, \omega) &= i \frac{\delta \bar{n}_1(\mathbf{q}, \omega)}{\tau_1}, \end{aligned}$$

whose solutions are readily obtainable:

$$\begin{aligned} \delta \bar{n}_1(\mathbf{q}, \omega) &= 2e v_F \sqrt{\frac{4\pi}{3}} \left(1 + \frac{F_1^S}{3} \right) \frac{-i \omega \tau}{i\omega - \frac{q^2 v_F^2 \tau}{3} (1 + F_0^S) \left(1 + \frac{F_1^S}{3} \right) + \omega^2 \tau} \mathcal{E}(\mathbf{q}, \omega), \\ \delta \bar{n}_0(\mathbf{q}, \omega) &= \sqrt{\frac{1}{3}} \frac{v_F q}{\omega} \left(1 + F_0^S \right) \delta \bar{n}_1(\mathbf{q}, \omega) \\ &= 2e v_F \frac{\sqrt{4\pi}}{3} \left(1 + \frac{F_1^S}{3} \right) \left(1 + F_0^S \right) \\ &\quad \times \frac{-i q v_F \tau}{i\omega - \frac{q^2 v_F^2 \tau}{3} (1 + F_0^S) \left(1 + \frac{F_1^S}{3} \right) + \omega^2 \tau} \mathcal{E}(\mathbf{q}, \omega). \end{aligned}$$

Therefore the electric current is found to be

$$\begin{aligned} J(\mathbf{q}, \omega) &= -e \frac{v_F}{2\sqrt{12\pi}} \mathcal{N} \delta \bar{n}_1(\mathbf{q}, \omega) \\ &= -e \frac{v_F}{2\sqrt{12\pi}} \mathcal{N} \left[\frac{-i \omega \tau 2e v_F \sqrt{\frac{4\pi}{3}} \left(1 + \frac{F_1^S}{3} \right)}{i\omega - \frac{q^2 v_F^2 \tau}{3} (1 + F_0^S) \left(1 + \frac{F_1^S}{3} \right) + \omega^2 \tau} \mathcal{E}(\mathbf{q}, \omega) \right] \end{aligned}$$

$$\begin{aligned}
&= \frac{n e^2 \tau}{m_*} \left(1 + \frac{F_1^S}{3}\right) \frac{i\omega}{i\omega - \frac{q^2 v_F^2 \tau}{3} (1 + F_0^S) \left(1 + \frac{F_1^S}{3}\right) + \omega^2 \tau} \mathcal{E}(\mathbf{q}, \omega) \\
&= \frac{n e^2 \tau}{m_*} \left(1 + \frac{F_1^S}{3}\right) \frac{i\omega}{i\omega - D q^2 + \omega^2 \tau} \mathcal{E}(\mathbf{q}, \omega) \\
&\equiv \sigma(\mathbf{q}, \omega) \mathcal{E}(\mathbf{q}, \omega),
\end{aligned} \tag{1.119}$$

where

$$D = \frac{v_F^2 \tau}{3} (1 + F_0^S) \left(1 + \frac{F_1^S}{3}\right), \tag{1.120}$$

is the diffusion coefficient.⁷ Seemingly, the charge density is

$$\begin{aligned}\delta\rho(\mathbf{q},\omega) &= \frac{1}{2\sqrt{4\pi}} \mathcal{N} \delta n_0(\mathbf{q},\omega) \\ &= \frac{1}{1+F_0^S} \mathcal{N} \frac{-iDq}{i\omega - Dq^2 + \omega^2\tau} e\mathcal{E}(\mathbf{q},\omega).\end{aligned}\quad (1.121)$$

We recall that, for a longitudinal field,

$$-e\mathcal{E}(\mathbf{q},\omega) = e i\mathbf{q}\phi(\mathbf{q},\omega) - i\frac{4\pi e^2}{q^2} \mathbf{q}\delta\rho(\mathbf{q},\omega) \equiv -i\mathbf{q}V(\mathbf{q},\omega),$$

⁷Indeed this behavior is characteristic of diffusive modes. If $\mathcal{E}(\mathbf{q},\omega) = 0$, the two coupled equations reduce to

$$\begin{aligned}-\frac{\omega}{1+F_0^S} \delta\bar{n}_0(\mathbf{q},\omega) + qv_F \sqrt{\frac{1}{3}} \delta\bar{n}_1(\mathbf{q},\omega) &= 0, \\ -\frac{\omega}{1+\frac{F_1^S}{3}} \delta\bar{n}_1(\mathbf{q},\omega) + qv_F \sqrt{\frac{1}{3}} \delta\bar{n}_0(\mathbf{q},\omega) &= i\frac{\delta\bar{n}_1(\mathbf{q},\omega)}{\tau_1},\end{aligned}$$

If we multiply the first by $\mathcal{N}/2\sqrt{4\pi}$, and the second by $\mathcal{N}v_F \left(1 + \frac{F_1^S}{3}\right)/2\sqrt{12\pi}$, we find

$$\begin{aligned}-\omega\delta\rho(\mathbf{q},\omega) + q\frac{J(\mathbf{q},\omega)}{-e} &= 0 \\ -\omega\frac{J(\mathbf{q},\omega)}{-e} + q\frac{D}{\tau}\delta\rho(\mathbf{q},\omega) &= i\frac{1}{\tau}\frac{J(\mathbf{q},\omega)}{-e}.\end{aligned}$$

The first equation is nothing but the continuity equation (the electric current is $-e$ times the charge current \mathbf{j}):

$$\frac{\partial\rho(\mathbf{x},t)}{\partial t} + \nabla \cdot \mathbf{j}(\mathbf{x},t) = 0.$$

The second equation for $\omega\tau \ll 1$, gives

$$j(\mathbf{q},\omega) = -iqD\delta\rho(\mathbf{q},\omega),$$

namely that the charge current,

$$\mathbf{j}(\mathbf{x},t) = -D\nabla\rho(\mathbf{x},t),$$

is proportional to minus the space-gradient of the charge density, the proportionality constant being the diffusion coefficient. Inserting this expression in the continuity equation, we find

$$\frac{\partial\rho(\mathbf{x},t)}{\partial t} - D\nabla^2\rho(\mathbf{x},t) = 0,$$

showing that charge diffuses with equation of motion

$$(-i\omega + Dq^2)\delta\rho(\mathbf{q},\omega) = 0.$$

where V is the internal scalar potential felt by the electrons. Therefore,

$$\delta\rho(\mathbf{q}, \omega) = \kappa \frac{D q^2}{i\omega - D q^2 + \omega^2 \tau} V(\mathbf{q}, \omega), \quad (1.122)$$

with κ the compressibility. This equation provides an expression of the “proper” response function in the presence of disorder

$$\chi_*(\mathbf{q}, \omega) = \kappa \frac{D q^2}{i\omega - D q^2 + \omega^2 \tau}, \quad (1.123)$$

hence of the “improper” one

$$\chi(\mathbf{q}, \omega) = \frac{\chi_*(\mathbf{q}, \omega)}{1 - \frac{4\pi e^2}{q^2} \chi_*(\mathbf{q}, \omega)}. \quad (1.124)$$

Chapter 2

Second Quantization

The first difficulty encountered in a many-body problem is how to deal with a many-body wavefunction. The reason is that a many-body wavefunction has to take into account both the indistinguishability of the particles and their statistics, while any operator, including the Hamiltonian, does not have in first quantization such properties. Hence it would be desirable to have at disposal an alternative scheme where the indistinguishability principle as well as the statistics of the particles were already built in the expression of the operators. This is actually the scope of second quantization.

2.1 Fock states and space

Let us take a system of N particles, either fermions or bosons. The Hilbert space spans a basis of N -body orthonormal wavefunctions which should satisfy both the indistinguishability principle as well as the appropriate statistics of the particles. The simplest way to construct this space is as follows.

We start by choosing an orthonormal basis of single particle wavefunctions:

$$\phi_a(x), \quad a = 1, 2, \dots \quad (2.1)$$

Here x is a generalized coordinate which include both the space coordinate \mathbf{x} as well as e.g. the z -component, σ , of the spin, which is half-integer for fermions and integer for bosons. The suffix a is a quantum label and

$$\begin{aligned} \int dx \phi_a(x)^* \phi_b(x) &= \delta_{ab} \\ \sum_a \phi_a(x)^* \phi_a(y) &= \delta(x - y). \end{aligned}$$

[The $\int dx \dots$ means $\sum_\sigma \int d\mathbf{x} \dots$, while $\delta(x - y) \equiv \delta(\mathbf{x} - \mathbf{y})\delta_{\sigma\sigma'}$ with $x = (\mathbf{x}, \sigma)$ and $y = (\mathbf{y}, \sigma')$]. A generic N -body wavefunction with the appropriate symmetry properties can be constructed

through the above single-particle states. Since the particles are not distinguishable, we do not need to know which particle occupies a specific state. Instead, what we need to know are just the occupation numbers n_a 's, i.e. the number of particles occupying each single-particle state ϕ_a . This number is either $n_a = 0, 1$ for fermions, because of Pauli principle, or an arbitrary integer $n_a \geq 0$ for bosons. Apart from that, the occupation numbers should satisfy the trivial particle-conservation constraint

$$\sum_a n_a = N.$$

Since the occupation numbers are the only ingredients we need in order to build up the N -body wave-function, we can formally denote the latter as the *ket*

$$|n_1, n_2, \dots\rangle, \quad (2.2)$$

which is called a *Fock state*, while the space spanned by the Fock states is called *Fock space*. Within the Fock space, the state with no particles, the vacuum, will be denoted by $|0\rangle$.

For instance, if the N fermions with coordinates x_i , $i = 1, \dots, N$, occupy the states a_j , $j = 1, \dots, N$, with $a_1 < a_2 < \dots < a_N$, namely $n_a = 1$ for $a \in \{a_j\}$, otherwise $n_a = 0$, then the appropriate wave-function is the Slater determinant

$$\Psi_{\{n_a\}}(x_1, \dots, x_N) = \sqrt{\frac{1}{N!}} \begin{vmatrix} \phi_{a_1}(x_1) & \cdots & \phi_{a_1}(x_N) \\ \phi_{a_2}(x_1) & \cdots & \phi_{a_2}(x_N) \\ \vdots & \ddots & \vdots \\ \phi_{a_N}(x_1) & \cdots & \phi_{a_N}(x_N) \end{vmatrix}, \quad (2.3)$$

which is therefore the first quantization expression of the Fock state $|\{n_a\}\rangle$ with the same occupation numbers. The above wave-function satisfies the condition of being anti-symmetric if two coordinates are interchanged, namely two columns in the determinant. Analogously, it is antisymmetric by interchanging two rows, i.e. two quantum labels.

On the contrary, if we have N bosons with coordinates x_i , $i = 1, \dots, N$, which occupy the states a_j , $j = 1, \dots, M$, $M \leq N$ and $a_1 < a_2 < \dots < a_M$, with occupation numbers n_{a_j} , then the appropriate wave-function is the permanent

$$\begin{aligned} \Phi_{\{n_a\}}(x_1, \dots, x_N) = & \sqrt{\frac{\prod_j n_j!}{N!}} \sum_p \phi_{a_1}(x_{p_1}) \dots \phi_{a_1}(x_{p_{n_{a_1}}}) \\ & \phi_{a_2}(x_{p_{n_{a_1}+1}}) \dots \phi_{a_2}(x_{p_{n_{a_1}+n_{a_2}}}) \dots \\ & \dots \phi_{a_M}(x_{p_{N-n_{a_M}+1}}) \dots \phi_{a_M}(x_{p_N}), \end{aligned} \quad (2.4)$$

where the sum is over all non-equivalent permutations p 's of the N coordinates¹. Indeed the wave-function is even by interchanging two coordinates or two quantum labels.

¹Non-equivalent means for instance that $\phi_i(x)\phi_i(y)$ is equivalent to $\phi_i(y)\phi_i(x)$

In conclusion, the space spanned by all possible Slater determinants built with the same basis set of single-particle wavefunctions constitutes an appropriate Hilbert (Fock) space for many-body fermionic wavefunctions. Analogously the space spanned by all possible permanents is an appropriate Hilbert space for many-body bosonic wavefunctions.

In the following we will introduce operators acting in the Fock space. We will consider separately the fermionic and bosonic cases.

2.2 Fermionic operators

Let us introduce the creation, c_a^\dagger , and annihilation, c_a , operators which add or remove, respectively, one fermion in state a . The operator $c_a^\dagger c_a$ first annihilates then creates a particle in a , which can be done as many times as many particles occupy that state. Therefore

$$c_a^\dagger c_a |n_a\rangle = n_a |n_a\rangle, \quad (2.5)$$

so it acts like the occupation number operator $c_a^\dagger c_a \equiv \hat{n}_a$. Since by Pauli principle $n_a = 0, 1$, then

$$c_a^\dagger c_a |0\rangle = 0, \quad c_a^\dagger c_a |n_a = 1\rangle = |n_a = 1\rangle. \quad (2.6)$$

Analogously, the operator $c_a c_a^\dagger$ first creates then destroys a fermion in state a , which can not do if a is occupied, while it can do once if empty. Therefore

$$c_a c_a^\dagger |0\rangle = |0\rangle, \quad c_a c_a^\dagger |n_a = 1\rangle = 0. \quad (2.7)$$

Thus, either a is empty or occupied, the following equation holds

$$(c_a c_a^\dagger + c_a^\dagger c_a) |n_a = 0, 1\rangle = |n_a = 0, 1\rangle,$$

which leads to the operator identity

$$(c_a c_a^\dagger + c_a^\dagger c_a) = \{c_a, c_a^\dagger\} = 1, \quad (2.8)$$

where the symbol $\{\dots\}$ means the anti-commutator. Moreover, since one can not create nor destroy two fermions in the same state, it also holds

$$\{c_a, c_a\} = \{c_a^\dagger, c_a^\dagger\} = 0. \quad (2.9)$$

Eqs. (2.8) and (2.9) are the anti-commutation relations satisfied by the fermion operators with the same quantum label. Going back to (2.6) and (2.7), we readily see that they are all satisfied if

$$c_a^\dagger |0\rangle = |n_a = 1\rangle, \quad c_a^\dagger |n_a = 1\rangle = 0$$

$$c_a|0\rangle = 0, \quad c_a|n_a = 1\rangle = |0\rangle,$$

also showing that c_a^\dagger is the hermitean conjugate of c_a .

Let us consider now the action of the above operators on a Fock state. Suppose we create two fermions, one in state a and one in b , with $a < b$. We can assume that

$$c_a^\dagger c_b^\dagger |0\rangle = |n_a = 1, n_b = 1\rangle, \quad c_b^\dagger c_a^\dagger |0\rangle = |n_b = 1, n_a = 1\rangle.$$

Since the two Fock states differ by interchanging two rows in the Slater determinant, then

$$|n_a = 1, n_b = 1\rangle = -|n_b = 1, n_a = 1\rangle,$$

hence

$$c_a^\dagger c_b^\dagger = -c_b^\dagger c_a^\dagger \rightarrow \{c_a^\dagger, c_b^\dagger\} = 0, \quad (2.10)$$

which is the third anticommutation relation. Analogously

$$\begin{aligned} c_a c_b^\dagger |n_a = 1\rangle &= c_a |n_b = 1, n_a = 1\rangle = -c_a |n_a = 1, n_b = 1\rangle = -|n_b = 1\rangle \\ c_b^\dagger c_a |n_a = 1\rangle &= c_b^\dagger |0\rangle = |n_b = 1\rangle, \end{aligned}$$

leading to the fourth anti-commutation relation

$$\{c_a, c_b^\dagger\} = 0. \quad (2.11)$$

They all can be cast in the general formulas

$$\{c_a, c_b^\dagger\} = \delta_{ab}, \quad \{c_a^\dagger, c_b^\dagger\} = 0, \quad \{c_a, c_b\} = 0. \quad (2.12)$$

Once we have introduced the above creation and annihilation operators, the Fock states have the simple expressions

$$|n_1, n_2, \dots\rangle = \prod_{i:n_i=1} c_i^\dagger |0\rangle, \quad (2.13)$$

where the product runs over all quantum labels i which correspond to occupied states.

2.2.1 Second quantization of multifermion-operators

Let us consider the single-particle operator in first quantization

$$\hat{V} = \sum_i V(x_i), \quad (2.14)$$

where the sum runs over all particles and $V(x_i)$ is an operator acting both on space coordinates and spins. We want to calculate the matrix element

$$\langle n'_1, n'_2, \dots | \hat{V} | n_1, n_2, \dots \rangle, \quad (2.15)$$

among two Slater determinants, equivalently Fock states, with occupation numbers n'_i 's and n_i 's, respectively. Since the operator \hat{V} conserves the number of particles, then

$$\sum_i n_i = \sum_j n'_j = N.$$

Being the particles not distinguishable, it derives that

$$\begin{aligned} \langle n'_1, n'_2, \dots | \hat{V} | n_1, n_2, \dots \rangle &= N \langle n'_1, n'_2, \dots | V(x_1) | n_1, n_2, \dots \rangle \\ &= \int dx_1 dx_2 \dots dx_N \Psi_{\{n'\}}(x_1, x_2, \dots, x_N)^* V(x_1) \Psi_{\{n\}}(x_1, x_2, \dots, x_N) \end{aligned}$$

We assume that in the Fock ket $|n_1, n_2, \dots\rangle$, the states a_i , $i = 1, \dots, N$ are occupied, with $a_1 < a_2 < \dots < a_N$, while in $|n'_1, n'_2, \dots\rangle$ are occupied b_j 's, $j = 1, \dots, N$. We can expand the Slater determinant in the first column, corresponding to particle x_1 and get

$$\Psi_{\{n\}}(x_1, x_2, \dots, x_N) = \frac{1}{\sqrt{N}} \sum_{i=1}^N (-1)^{i-1} \phi_{a_i}(x_1) \Psi_{\{n: n_{a_i}=0\}}(x_2, \dots, x_N),$$

where $\Psi_{\{n: n_{a_i}=0\}}(x_2, \dots, x_N)$ is the Slater determinant of the $N - 1$ particles x_2, x_3, \dots, x_N with the same occupation numbers as $\Psi_{\{n\}}(x_1, x_2, \dots, x_N)$ apart from state a_i which is empty. Analogously

$$\Psi_{\{n'\}}(x_1, x_2, \dots, x_N)^* = \frac{1}{\sqrt{N}} \sum_{j=1}^N (-1)^{j-1} \phi_{b_j}(x_1)^* \Psi_{\{n': n_{b_j}=0\}}(x_2, \dots, x_N)^*.$$

Therefore

$$\begin{aligned} \langle n'_1, n'_2, \dots | \hat{V} | n_1, n_2, \dots \rangle &= \\ \sum_{i,j} (-1)^{i+j} \int dx_1 \phi_{b_j}(x_1)^* V(x_1) \phi_{a_i}(x_1) \langle n'_1, n'_2, \dots, n_{b_j} - 1, \dots | n_1, n_2, \dots, n_{a_i} - 1, \dots \rangle &= \\ \sum_{i,j} (-1)^{i+j} V_{b_j, a_i} \prod_{k \neq a_i, b_j} \delta_{n_k, n'_k}. & \end{aligned} \tag{2.16}$$

One easily realizes that the same result is obtained if, instead of using the first quantization expression (2.14), one uses

$$\hat{V} = \sum_{i,j} V_{i,j} c_i^\dagger c_j, \tag{2.17}$$

where

$$V_{i,j} = \int dx \phi_i(x)^* V(x) \phi_j(x). \quad ^2$$

²Notice that if the operator $V(x)$ acts on the spins, namely $V(x) \rightarrow V_{\sigma\sigma'}(\mathbf{x})$, then

$$V_{i,j} = \sum_{\sigma\sigma'} \int d\mathbf{x} \phi_i(\mathbf{x}, \sigma)^* V_{\sigma\sigma'}(\mathbf{x}) \phi_j(\mathbf{x}, \sigma').$$

Let us continue and consider a two particle operator

$$\hat{U} = \frac{1}{2} \sum_{i \neq j} U(x_i, x_j). \quad (2.18)$$

The matrix element between two Fock states is now

$$\langle n'_1, n'_2, \dots | \hat{U} | n_1, n_2, \dots \rangle = \frac{N(N-1)}{2} \langle n'_1, n'_2, \dots | U(x_1, x_2) | n_1, n_2, \dots \rangle \quad (2.19)$$

In this case we need to expand the Slater determinants in the first two columns:

$$\begin{aligned} \Psi_{\{n\}}(x_1, x_2, \dots, x_N) &= \frac{1}{\sqrt{N(N-1)}} \sum_{i \neq j=1}^N (-1)^{i-1} (-1)^{j-1-\theta_{j,i}} \phi_{a_j}(x_2) \phi_{a_i}(x_1) \\ &\quad \Psi_{\{n: n_{a_i}=0, n_{a_j}=0\}}(x_3, \dots, x_N), \end{aligned} \quad (2.20)$$

where now $\Psi_{\{n: n_{a_i}=0, n_{a_j}=0\}}(x_3, \dots, x_N)$ is the Slater determinant of the $N-2$ particles x_3, x_4, \dots, x_N in which, differently from $\Psi_{\{n\}}(x_1, x_2, \dots, x_N)$, the states a_i and a_j are empty. The $\theta_{j,i}$ function is = 1 if $j > i$ and = 0 if $j < i$. Analogously

$$\begin{aligned} \Psi_{\{n'\}}(x_1, x_2, \dots, x_N)^* &= \frac{1}{\sqrt{N(N-1)}} \sum_{i \neq j=1}^N (-1)^{i-1} (-1)^{j-1-\theta_{j,i}} \phi_{b_i}^*(x_1)^* \phi_{b_j}^*(x_2)^* \\ &\quad \Psi_{\{n: n_{b_i}=0, n_{b_j}=0\}}(x_3, \dots, x_N)^*. \end{aligned} \quad (2.21)$$

Therefore

$$\begin{aligned} \frac{N(N-1)}{2} \langle n'_1, n'_2, \dots | U(x_1, x_2) | n_1, n_2, \dots \rangle &= \frac{1}{2} \sum_{i \neq j=1}^N \sum_{m \neq l=1}^N (-1)^{i+j+\theta_{j,i}} (-1)^{m+n+\theta_{n,m}} \\ &\quad \int dx_1 dx_2 \phi_{b_m}^*(x_1)^* \phi_{b_n}^*(x_2)^* U(x_1, x_2) \phi_{a_j}(x_2) \phi_{a_i}(x_1) \\ &\quad \int dx_3 \dots dx_N \Psi_{\{n: n_{b_m}=0, n_{b_n}=0\}}(x_3, \dots, x_N)^* \Psi_{\{n: n_{a_i}=0, n_{a_j}=0\}}(x_3, \dots, x_N) \\ &= \frac{1}{2} \sum_{i \neq j=1}^N \sum_{m \neq l=1}^N (-1)^{i+j+\theta_{j,i}} (-1)^{m+n+\theta_{n,m}} U_{b_m, b_n; a_j, a_i} \prod_{l \neq a_i, a_j, b_m, b_n} \delta_{n'_l, n_l}. \end{aligned} \quad (2.22)$$

It is a straightforward calculation to show that the same expression is obtained if

$$\hat{U} = \frac{1}{2} \sum_{ijkl} U_{i,j;k,l} c_i^\dagger c_j^\dagger c_k c_l, \quad (2.23)$$

where

$$U_{i,j;k,l} = \int dx dy \phi_i(x)^* \phi_j(y)^* U(x,y) \phi_k(y) \phi_l(x).$$

Analogously, one can introduce m -particle operators

$$\hat{U}_m = \frac{1}{m!} \sum_{i_1 \neq i_2 \neq \dots \neq i_m} U(x_1, x_2, \dots, x_m),$$

which translate in second quantization language into

$$\begin{aligned} \hat{U}_m &= \frac{1}{m!} \sum_{i_1, j_1, i_2, j_2, \dots, i_m, j_m} U_{i_1, i_2, \dots, i_m; j_m, j_{m-1}, \dots, j_1} \\ &\quad c_{i_1}^\dagger c_{i_2}^\dagger \dots c_{i_m}^\dagger c_{j_m} c_{j_{m-1}} \dots c_{j_1}, \end{aligned} \quad (2.24)$$

with

$$\begin{aligned} U_{i_1, i_2, \dots, i_m; j_m, j_{m-1}, \dots, j_1} &= \int dx_1 dx_2 \dots dx_m \phi_{i_1}(x_1)^* \phi_{i_2}(x_2)^* \dots \phi_{i_m}(x_m)^* \\ &\quad U(x_1, x_2, \dots, x_m) \phi_{j_m}(x_m) \phi_{j_{m-1}}(x_{m-1}) \dots \phi_{j_1}(x_1). \end{aligned}$$

We conclude by emphasizing the advantages of second quantization with respect to first quantization. In the former, any multiparticle operator depends explicitly on the particle coordinates. It is only the wave-function which contains information about either the indistinguishability of the particles as well as their statistics. On the contrary, in second quantization those properties are hidden in the definition of creation and annihilation operators, hence the multiparticle operators do not depend anymore on the particle coordinates. Moreover in second quantization we can also introduce operators which have no first-quantization counterpart. For instance we can define particle-non-conserving operators which connect subspaces with different numbers of particles of the whole Hilbert space. For instance

$$\sum_{i,j} \Delta_{i,j} c_i^\dagger c_j^\dagger + \Delta_{i,j}^* c_j c_i,$$

is an operator which connects Fock states with particle numbers differing by two. As we shall see such operators are useful for discussing superconductivity.

2.2.2 Fermi fields

Till now we have defined fermionic operators for a given set of single-particle wavefunctions. Let us now introduce new operators which are independent of this choice. We define annihilation and creation Fermi fields by

$$\Psi_\sigma(\mathbf{x}) \equiv \Psi(x) = \sum_i \phi_i(x) c_i, \quad \Psi(x)^\dagger = \sum_i \phi_i(x)^* c_i^\dagger. \quad (2.25)$$

They satisfy the following properties

$$\begin{aligned}\{\Psi(x), \Psi(y)^\dagger\} &= \sum_{ij} \phi_i(x) \phi_j(y)^* \{c_i, c_j^\dagger\} \\ &= \sum_i \phi_i(x) \phi_i(y)^* = \delta(x - y),\end{aligned}\quad (2.26)$$

as well as

$$\{\Psi(x), \Psi(y)\} = \{\Psi(x)^\dagger, \Psi(y)^\dagger\} = 0. \quad (2.27)$$

which are indeed independent upon the basis. If we change the basis via the unitary transformation \hat{U} acting on the basis set

$$\phi_i(x) = \sum_\alpha U_{\alpha,i} \phi_\alpha(x),$$

with $\hat{U}\hat{U}^\dagger = \mathcal{I}$, the identity matrix, then

$$\begin{aligned}\Psi(x) &= \sum_i \phi_i(x) c_i = \sum_{i,\alpha} \phi_\alpha(x) U_{\alpha,i} c_i \\ &= \sum_\alpha \phi_\alpha(x) c_\alpha,\end{aligned}\quad (2.28)$$

showing the proper transformation properties of the fermionic operators

$$c_\alpha = \sum_i U_{\alpha,i} c_i. \quad (2.29)$$

The multiparticle operators in second quantization have a very simple expression in terms of the Fermi fields. For instance it is easy to show that Eq. (2.17) can also be written as

$$\hat{V} = \sum_{ij} V_{i,j} c_i^\dagger c_j = \int dx \Psi(x)^\dagger V(x) \Psi(x), \quad (2.30)$$

and analogously (2.23) as

$$\hat{U} = \frac{1}{2} \sum_{ijkl} U_{i,j;k,l} c_i^\dagger c_j^\dagger c_k c_l = \frac{1}{2} \int dx dy \Psi(x)^\dagger \Psi(y)^\dagger U(x, y) \Psi(y) \Psi(x), \quad (2.31)$$

and finally (2.24) as

$$\hat{U}_m = \frac{1}{m!} \sum_{i_1, j_1, i_2, j_2, \dots, i_m, j_m} U_{i_1, i_2, \dots, i_m; j_m, j_{m-1}, \dots, j_1}$$

$$c_{i_1}^\dagger c_{i_2}^\dagger \dots c_{i_m}^\dagger c_{j_m} c_{j_{m-1}} \dots c_{j_1} \\ = \frac{1}{m!} \int dx_1 \dots dx_m \Psi(x_1)^\dagger \dots \Psi(x_m)^\dagger U(x_1, \dots, x_m) \Psi(x_m) \dots \Psi(x_1). \quad (2.32)$$

Let us for instance consider the density operator in first quantization

$$\hat{\rho}_\sigma(\mathbf{x}) = \sum_{i=1}^N \delta(\mathbf{x} - \mathbf{x}_i) \delta_{\sigma, \sigma_i}.$$

In second quantization, through Eq. (2.30), it reads

$$\begin{aligned} \hat{\rho}_\sigma(\mathbf{x}) &= \sum_{\sigma'} \int d\mathbf{y} \Psi_{\sigma'}(\mathbf{y})^\dagger \delta(\mathbf{x} - \mathbf{y}) \delta_{\sigma, \sigma'} \Psi_{\sigma'}(\mathbf{y}) \\ &= \Psi_\sigma(\mathbf{x})^\dagger \Psi_\sigma(\mathbf{x}) = \Psi(x)^\dagger \Psi(x), \end{aligned} \quad (2.33)$$

which also shows that $\Psi(x)^\dagger$ is nothing but the operator which creates a particle in coordinate x , while $\Psi(x)$ destroys it.

2.3 Bosonic operators

As previously done for the fermionic case, we introduce the creation, d_a^\dagger , and its hermitean conjugate, the annihilation d_a , operators which respectively create and destroy a boson in state a . Again the operators $d_a^\dagger d_a$ counts how many times we can destroy and create back a boson in state a , hence it is just the occupation number n_a . However, since Pauli principle does not hold for bosons, the operator $d_a d_a^\dagger$ first adds one boson in state a , hence increases $n_a \rightarrow n_a + 1$, then destroys one in the same state. This latter process can be done $n_a + 1$ times, being $n_a + 1$ the actual occupation number once one more boson has been added. Therefore

$$d_a^\dagger d_a |n_a\rangle = n_a |n_a\rangle, \quad d_a d_a^\dagger |n_a\rangle = (1 + n_a) |n_a\rangle, \quad (2.34)$$

hence the following commutation relation holds

$$[d_a, d_a^\dagger] = d_a d_a^\dagger - d_a^\dagger d_a = 1, \quad (2.35)$$

where $[\dots]$ denotes the commutator. Eq. (2.34) is trivially satisfied by

$$d_a |n_a\rangle = \sqrt{n_a} |n_a - 1\rangle, \quad d_a^\dagger |n_a\rangle = \sqrt{n_a + 1} |n_a + 1\rangle. \quad (2.36)$$

The permanent, contrary to the Slater determinant, is invariant upon interchanging two quantum labels. As a consequence, bosonic operators corresponding to different states commute instead of anti-commuting as the fermionic ones. Namely, for $a \neq b$,

$$[d_a^\dagger, d_b] = [d_a^\dagger, d_b^\dagger] = 0.$$

Therefore, in general,

$$[d_a, d_b^\dagger] = \delta_{ab}, \quad [d_a^\dagger, d_b^\dagger] = [d_a, d_b] = 0. \quad (2.37)$$

Moreover, through (2.36) and (2.37) we can write a generic Fock state as

$$|n_1, n_2, \dots\rangle = \prod_i \frac{(d_i^\dagger)^{n_i}}{\sqrt{n_i!}} |0\rangle. \quad (2.38)$$

2.3.1 Bose fields and multiparticle operators

The analogous role of the Fermi fields is now played by the Bose fields defined through

$$\Phi(x) = \sum_a \phi_a(x) d_a, \quad \Phi(x)^\dagger = \sum_a \phi_a(x)^* d_a^\dagger, \quad (2.39)$$

which satisfy the commutation relations

$$[\Phi(x), \Phi(y)^\dagger] = \delta(x - y), \quad [\Phi(x), \Phi(y)] = [\Phi(x)^\dagger, \Phi(y)^\dagger] = 0, \quad (2.40)$$

Let us consider the expansion of the permanent (2.4) over e.g. the coordinate x_1 . One can easily show that it is given by

$$\begin{aligned} |n_1, n_2, \dots\rangle &= \Phi_{\{n\}}(x_1, x_2, \dots, x_N) = \sum_a \sqrt{\frac{n_a}{N}} \phi_a(x_1) \Phi_{\{n:n_a \rightarrow n_a-1\}}(x_2, \dots, x_N) \\ &= \sum_a \sqrt{\frac{n_a}{N}} \phi_a(x_1) |n_1, n_2, \dots, n_a - 1, \dots\rangle, \end{aligned} \quad (2.41)$$

where the $\sqrt{n_a}$ also enforces that the sum does not include empty states. By means of (2.41) we can write the matrix element of a single-particle operator like (2.14) as

$$\begin{aligned} \langle n'_1, n'_2, \dots | \hat{V} | n_1, n_2, \dots \rangle &= N \langle n'_1, n'_2, \dots | V(x_1) | n_1, n_2, \dots \rangle \\ &= \sum_{ab} \sqrt{n_a n'_b} \int dx_1 \phi_b(x_1)^* V(x_1) \phi_a(x_1) \langle n'_1, n'_2, \dots, n'_b - 1, \dots | n_1, n_2, \dots, n_a - 1, \dots \rangle \\ &= \langle n'_1, n'_2, \dots | \int dx \Phi(x)^\dagger V(x) \Phi(x) | n_1, n_2, \dots \rangle, \end{aligned}$$

thus showing that

$$\hat{V} = \int dx \Phi(x)^\dagger V(x) \Phi(x). \quad (2.42)$$

Analogously we can expand the permanent in two coordinates, e.g. x_1 and x_2 ,

$$|n_1, n_2, \dots\rangle = \Phi_{\{n\}}(x_1, x_2, \dots, x_N) =$$

$$\sum_{ab} \sqrt{\frac{n_a}{N}} \sqrt{\frac{n_b - \delta_{ab}}{N-1}} \phi_b(x_2) \phi_a(x_1) \Phi_{\{n:n_a \rightarrow n_a-1:n_b \rightarrow n_b-1\}}(x_3, \dots, x_N),$$

and show that the average of a two-body interaction like (2.18) can be written as

$$\begin{aligned} \langle n'_1, n'_2, \dots | \hat{U} | n_1, n_2, \dots \rangle &= \frac{N(N-1)}{2} \langle n'_1, n'_2, \dots | U(x_1, x_2) | n_1, n_2, \dots \rangle \\ &= \frac{1}{2} \sum_{abcd} \sqrt{n'_a(n'_b - \delta_{ab})n_d(n_c - \delta_{cd})} \int dx_1 dx_2 \phi_a(x_1)^* \phi_b(x_2)^* U(x_1, x_2) \phi_c(x_2) \phi_d(x_1) \\ &\quad \langle n'_1, n'_2, \dots, n'_a - 1, \dots, n'_b - 1, \dots | n_1, n_2, \dots, n_c - 1, \dots, n_d - 1, \dots \rangle. \end{aligned}$$

Therefore, like in the fermionic case, we can formally identify

$$\hat{U} = \frac{1}{2} \int dx dy \Phi(x)^\dagger \Phi(y)^\dagger U(x, y) \Phi(y) \Phi(x), \quad (2.43)$$

as well as for the m -particle operators

$$\hat{U}_m = \frac{1}{m!} \int dx_1 \dots dx_m \Phi(x_1)^\dagger \dots \Phi(x_m)^\dagger U(x_1, \dots, x_m) \Phi(x_m) \dots \Phi(x_1). \quad (2.44)$$

2.4 Canonical transformations

In general an interacting Hamiltonian, which contains besides bilinear also quartic and higher order terms in creation and annihilation operators, can not be diagonalized. On the contrary, a bilinear Hamiltonian is diagonalizable by a canonical transformation.

A canonical transformation preserves the commutation/anti-commutation properties of the operators.

Since the interaction is commonly analysed perturbatively starting from an appropriate non-interacting theory, it is useful to begin with bilinear Hamiltonians and introduce the canonical transformations which diagonalize them.

The simplest bilinear Hamiltonian is the second quantized expression of a non-interacting first-quantization Hamiltonian, which has the general form

$$\hat{H} = \sum_{ab} t_{ab} c_a^\dagger c_b, \quad (2.45)$$

both for fermions and bosons. Since \hat{H} is hermitean, then

$$t_{ab} = t_{ba}^*.$$

If \tilde{t} is the hermitean matrix with elements t_{ab} , there exists a unitary transformation \tilde{U} , $\tilde{U} \tilde{U}^\dagger = \tilde{I}$, with \tilde{I} the identity matrix, such that

$$\sum_{ab} U_{\alpha a}^\dagger t_{ab} U_{b\beta} = \epsilon_\alpha \delta_{\alpha\beta}. \quad (2.46)$$

Therefore, if we define

$$c_a = \sum_\alpha U_{a\alpha} c_\alpha, \quad (2.47)$$

then through (2.46) we find

$$\hat{H} = \sum_{\alpha\beta} \sum_{ab} c_\alpha^\dagger U_{\alpha a}^\dagger t_{ab} U_{b\beta} c_\beta = \sum_\alpha \epsilon_\alpha c_\alpha^\dagger c_\alpha. \quad (2.48)$$

We have now to check whether the above is a canonical transformation. If the c_α 's are fermionic/bosonic operators then

$$\{c_a, c_b^\dagger\}_\pm = \sum_{\alpha\beta} U_{a\alpha} U_{\beta b}^\dagger \{c_\alpha, c_\beta^\dagger\}_\pm = \sum_\alpha U_{a\alpha} U_{\alpha b}^\dagger = \delta_{ab},$$

where $\{\dots\}_\pm$ stands for the anticommutator (+) and commutator (-), respectively. Therefore also the c_a 's are fermions/bosons, hence \hat{U} is indeed canonical.

Once the Hamiltonian has been transformed into the diagonal form (2.48), the problem is solved. Indeed any Fock state constructed through the new basis set with operators c_α , namely a wave-function $|\{n_\alpha\}\rangle$ where each state α is occupied by n_α particles, is an eigenstate of the Hamiltonian

$$\hat{H} |\{n_\alpha\}\rangle = \left[\sum_\alpha \epsilon_\alpha n_\alpha \right] |\{n_\alpha\}\rangle.$$

2.4.1 More general canonical transformations

In second quantization we have the opportunity to introduce bilinear Hamiltonians which does not conserve the number of particles:

$$\hat{H} = \sum_{ab} t_{ab} c_a^\dagger c_b + \Delta_{ab} c_a c_b + \Delta_{ab}^* c_b^\dagger c_a^\dagger. \quad (2.49)$$

These Hamiltonians are relevant for a wide class of physical problems. Again $t_{ab} = t_{ba}^*$ while

$$\Delta_{ab} = -\Delta_{ba}$$

for fermions, and for bosons

$$\Delta_{ab} = \Delta_{ba}.$$

The most general transformation which may diagonalize the Hamiltonian is of the form

$$c_a = \sum_{\alpha} U_{a\alpha} c_{\alpha} + V_{a\alpha} c_{\alpha}^{\dagger}, \quad (2.50)$$

$$c_a^{\dagger} = \sum_{\alpha} U_{a\alpha}^* c_{\alpha}^{\dagger} + V_{a\alpha}^* c_{\alpha}. \quad (2.51)$$

Let us derive the conditions under which the above is a canonical transformation:

$$\begin{aligned} \{c_a, c_b^{\dagger}\}_{\pm} &= \sum_{\alpha\beta} U_{a\alpha} U_{\beta b}^{\dagger} \{c_{\alpha}, c_{\beta}^{\dagger}\}_{\pm} + V_{a\alpha} V_{\beta b}^{\dagger} \{c_{\alpha}^{\dagger}, c_{\beta}\}_{\pm} \\ &= \sum_{\alpha} U_{a\alpha} U_{\alpha b}^{\dagger} \pm V_{a\alpha} V_{\alpha b}^{\dagger} \equiv \delta_{ab} \\ \{c_a, c_b\}_{\pm} &= \sum_{\alpha\beta} U_{a\alpha} V_{b\beta} \{c_{\alpha}, c_{\beta}^{\dagger}\}_{\pm} + V_{a\alpha} U_{b\beta} \{c_{\alpha}^{\dagger}, c_{\beta}\}_{\pm} \\ &= \sum_{\alpha} U_{a\alpha} V_{b\alpha} \pm V_{a\alpha} U_{b\alpha} \equiv 0. \end{aligned}$$

This implies that, for fermions

$$\tilde{U} \tilde{U}^{\dagger} + \tilde{V} \tilde{V}^{\dagger} = \tilde{I}, \quad \tilde{U} \tilde{V}^T + \tilde{V} \tilde{U}^T = 0, \quad (2.52)$$

while, for bosons,

$$\tilde{U} \tilde{U}^{\dagger} - \tilde{V} \tilde{V}^{\dagger} = \tilde{I}, \quad \tilde{U} \tilde{V}^T - \tilde{V} \tilde{U}^T = 0. \quad (2.53)$$

In addition, \tilde{U} and \tilde{V} should diagonalize (2.49), namely, once we write the original c_a 's and c_a^{\dagger} 's in terms of the new operators, we should obtain

$$\hat{H} = \sum_{\alpha} \epsilon_{\alpha} c_{\alpha}^{\dagger} c_{\alpha}.$$

We conclude by pointing out that, due to the particle-non-conserving terms, the vacuum of the original particles, $|0\rangle$, is no more the vacuum of the new ones, $|\tilde{0}\rangle$. Indeed

$$c_a |\tilde{0}\rangle = \sum_{\alpha} V_{a\alpha} c_{\alpha}^{\dagger} |\tilde{0}\rangle \neq 0.$$

2.5 Examples and Exercises

Let us consider electrons in a square box of linear length L with periodic boundary conditions. As a basis of single-particle wave-functions we use simple plane waves and spinors, namely the quantum label $a = (\mathbf{k}, s)$ with

$$\mathbf{k} = \frac{2\pi}{L} (n_x, n_y, n_z),$$

being n_i 's integers, $s = \pm 1/2 = \uparrow, \downarrow$. Hence the single-particle wavefunctions of the basis set are

$$\phi_a(\mathbf{x}) = \frac{1}{\sqrt{L^3}} e^{i\mathbf{k}\cdot\mathbf{x}} \delta_{s\sigma}.$$

The annihilation and creation operators are defined as

$$c_{\mathbf{k}\sigma}, \quad c_{\mathbf{k}\sigma}^\dagger,$$

hence the Fermi fields are

$$\begin{aligned} \Psi_\sigma(\mathbf{x}) &= \frac{1}{\sqrt{L^3}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} c_{\mathbf{k}\sigma}, \\ \Psi_\sigma^\dagger(\mathbf{x}) &= \frac{1}{\sqrt{L^3}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{x}} c_{\mathbf{k}\sigma}^\dagger. \end{aligned}$$

Let us start from the kinetic energy, which is in first quantization

$$\mathcal{H}_{kin} = \sum_{i=1}^N -\frac{\hbar^2}{2m} \nabla_i^2,$$

diagonal in the spin coordinate. Since

$$\frac{1}{L^3} \int d\mathbf{x} e^{-i\mathbf{k}\cdot\mathbf{x}} \left(-\frac{\hbar^2}{2m} \nabla^2 \right) e^{i\mathbf{p}\cdot\mathbf{x}} = \frac{\hbar^2 k^2}{2m} \delta_{\mathbf{k}\mathbf{p}},$$

then, in the plane-wave basis, the kinetic energy in second quantization becomes

$$\mathcal{H}_{kin} = \sum_{\mathbf{k}\sigma} \frac{\hbar^2 k^2}{2m} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \equiv \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}. \quad (2.54)$$

The ground state with N , assumed to be even, electrons is the Fermi sea $|FS\rangle$ obtained by filling with a spin-up and spin-down electrons the lowest energy levels up to the Fermi momentum k_F defined through

$$N = 2 \sum_{|\mathbf{k}| \leq k_F},$$

namely

$$|FS\rangle = \prod_{\mathbf{k}:|\mathbf{k}| \leq k_F} c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\downarrow}^\dagger |0\rangle, \quad (2.55)$$

hence the occupation number in momentum space is

$$n_{\mathbf{k}\uparrow} = n_{\mathbf{k}\downarrow} = \theta(k_F - |\mathbf{k}|),$$

where the θ -function is defined through $\theta(x) = 1$ if $x \geq 0$, otherwise $\theta(x) = 0$.

Let us add an electron-electron interaction of the general form

$$\mathcal{H}_{int} = \frac{1}{2} \sum_{i \neq j} V(\mathbf{x}_i - \mathbf{x}_j).$$

In second quantization it becomes

$$\begin{aligned} \mathcal{H}_{int} &= \frac{1}{2} \sum_{\sigma\sigma'} \int d\mathbf{x} d\mathbf{y} \Psi_\sigma^\dagger(\mathbf{x}) \Psi_{\sigma'}^\dagger(\mathbf{y}) V(\mathbf{x} - \mathbf{y}) \Psi_{\sigma'}(\mathbf{y}) \Psi_\sigma(\mathbf{x}) \\ &= \frac{1}{2L^3} \sum_{\sigma\sigma'} \sum_{\mathbf{k}_i, i=1,\dots,4} c_{\mathbf{k}_1\sigma}^\dagger c_{\mathbf{k}_2\sigma'}^\dagger c_{\mathbf{k}_3\sigma'} c_{\mathbf{k}_4\sigma} \frac{1}{L^3} \int d\mathbf{x} d\mathbf{y} e^{-i\mathbf{k}_1 \cdot \mathbf{x}} e^{-i\mathbf{k}_2 \cdot \mathbf{y}} e^{i\mathbf{k}_3 \cdot \mathbf{y}} e^{i\mathbf{k}_4 \cdot \mathbf{x}} V(\mathbf{x} - \mathbf{y}). \end{aligned}$$

We define the Fourier transform of the potential as

$$V(\mathbf{q}) = \int d\mathbf{r} e^{-i\mathbf{q} \cdot \mathbf{r}} V(\mathbf{r}),$$

so that

$$V(\mathbf{x} - \mathbf{y}) = \frac{1}{L^3} \sum_{\mathbf{q}} e^{i\mathbf{q} \cdot (\mathbf{x} - \mathbf{y})} V(\mathbf{q}),$$

and the interaction is finally found to be

$$\mathcal{H}_{int} = \frac{1}{L^3} \sum_{\sigma\sigma'} \sum_{\mathbf{k} \mathbf{p} \mathbf{q}} V(\mathbf{q}) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{p}+\mathbf{q}\sigma'}^\dagger c_{\mathbf{p}\sigma'} c_{\mathbf{k}+\mathbf{q}\sigma}. \quad (2.56)$$

We showed that the electron density for spin σ in second quantization is

$$\rho_\sigma(\mathbf{x}) = \Psi_\sigma^\dagger(\mathbf{x}) \Psi_\sigma(\mathbf{x}).$$

Its Fourier transform is

$$\rho_\sigma(\mathbf{q}) = \int d\mathbf{x} e^{-i\mathbf{q} \cdot \mathbf{x}} \Psi_\sigma^\dagger(\mathbf{x}) \Psi_\sigma(\mathbf{x}) = \sum_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}+\mathbf{q}\sigma}.$$

Let us consider interacting electrons also in the presence of a single-particle potential, provided e.g. by the ions,

$$\mathcal{H}_{pot} = \sum_{\sigma} \int d\mathbf{x} U(\mathbf{x}) \rho_{\sigma}(\mathbf{x}),$$

so that the total Hamiltonian reads

$$\mathcal{H} = \mathcal{H}_{kin} + \mathcal{H}_{int} + \mathcal{H}_{pot}.$$

Since the Hamiltonian conserves the total number of electrons, the electron density summed over the spins, i.e. $\rho = \rho_{\uparrow} + \rho_{\downarrow}$ must satisfy a continuity equation. Let us define the Heisenberg evolution of the density through

$$\rho(x, t) = e^{i\mathcal{H}t} \rho(x) e^{-i\mathcal{H}t}.$$

Since the integral of the density over the whole volume is the total number of electrons, N , which is conserved, it follows that

$$\int d\mathbf{x} \frac{\partial \rho(\mathbf{x}, t)}{\partial t} = \frac{\partial}{\partial t} \int d\mathbf{x} \rho(\mathbf{x}, t) = \frac{\partial N}{\partial t} \equiv 0.$$

This condition is satisfied if

$$\frac{\partial \rho(\mathbf{x}, t)}{\partial t} = -\nabla \mathbf{J}(\mathbf{x}, t),$$

where $\mathbf{J}(\mathbf{x}, t)$ is the current density operator. In fact, the integral over the volume of the left hand side is also equal to minus the flux of the current through the surface of the sample. If the number of electrons is conserved, it means that the flux of the current through the surface vanishes, which is the desired result.

Exercises:

- Calculate the formal expression of the average value of

$$\mathcal{H} = \mathcal{H}_{kin} + \mathcal{H}_{int},$$

over the Fermi sea wave-function (2.55);

- Using the Heisenberg equation of motion of the operators, according to which

$$i\hbar \frac{\partial \rho(\mathbf{x}, t)}{\partial t} = [\rho(\mathbf{x}, t), \mathcal{H}],$$

calculate the expression of the Fourier transform of the current $\mathbf{J}(\mathbf{q})$;

- Calculate the following commutator

$$[\rho(\mathbf{q}, t), \mathbf{J}(-\mathbf{q}, t)], \tag{2.57}$$

which is commonly known as the *f*-sum rule.

2.6 Application: fermionic lattice models and the emergence of magnetism

Let us consider the electron Hamiltonian in the presence of the periodic potential provided by the ions in a lattice:

$$\begin{aligned}\mathcal{H} &= \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m} + \sum_i \sum_{\mathbf{R}} V(\mathbf{x}_i - \mathbf{R}) + \frac{1}{2} \sum_{i \neq j} U(\mathbf{x}_i - \mathbf{x}_j) \\ &= \mathcal{H}_{kin} + \mathcal{H}_{el-ion} + \mathcal{H}_{el-el} = \mathcal{H}_0 + \mathcal{H}_{el-el},\end{aligned}\quad (2.58)$$

where \mathbf{R} are lattice vectors. We start by rewriting the Hamiltonian in second quantization. For that purpose we need to introduce a basis set of single-particle wavefunctions. Since the Hamiltonian is spin independent, it is convenient to work with factorized single-particle wavefunctions: $\phi(\mathbf{x}, \sigma) = \phi(\mathbf{x}) \chi_\sigma$. As a basis for the space-dependent $\phi(\mathbf{x})$ we use Wannier wave-functions $\phi(\mathbf{x})_{n,\mathbf{R}}$ satisfying the usual conditions

$$\int d\mathbf{x} \phi(\mathbf{x})_{n,\mathbf{R}_1}^* \phi(\mathbf{x})_{m,\mathbf{R}_2} = \delta_{nm} \delta_{\mathbf{R}_1 \mathbf{R}_2}, \quad \sum_{n,\mathbf{R}} \phi(\mathbf{x})_{n,\mathbf{R}}^* \phi(\mathbf{y})_{n,\mathbf{R}} = \delta(\mathbf{x} - \mathbf{y}),$$

as well as

$$\phi(\mathbf{x})_{n,\mathbf{R}+\mathbf{R}_0} = \phi(\mathbf{x} - \mathbf{R}_0)_{n,\mathbf{R}}. \quad (2.59)$$

Consequently we associate to any wavefunction $\phi(\mathbf{x})_{n,\mathbf{R}} \chi_\sigma$ creation, $c_{n,\mathbf{R},\sigma}^\dagger$, and annihilation, $c_{n,\mathbf{R},\sigma}$, operators, and introduce the Fermi fields

$$\Psi_\sigma(\mathbf{x}) = \sum_{n,\mathbf{R}} \phi(\mathbf{x})_{n,\mathbf{R}} c_{n,\mathbf{R},\sigma}, \quad \Psi_\sigma^\dagger(\mathbf{x}) = (\Psi_\sigma(\mathbf{x}))^\dagger.$$

Let us start by second quantization of the non interacting part of the Hamiltonian, \mathcal{H}_0 in Eq. (2.58):

$$\begin{aligned}\mathcal{H}_0 &= \sum_\sigma \int d\mathbf{x} \Psi_\sigma^\dagger(\mathbf{x}) \left[-\frac{\hbar^2 \nabla^2}{2m} + \sum_{\mathbf{R}} V(\mathbf{x} - \mathbf{R}) \right] \Psi_\sigma(\mathbf{x}) \\ &= \sum_\sigma \sum_{nm} \sum_{\mathbf{R}_1, \mathbf{R}_2} t_{\mathbf{R}_1, \mathbf{R}_2}^{nm} c_{n, \mathbf{R}_1, \sigma}^\dagger c_{m, \mathbf{R}_2, \sigma}.\end{aligned}\quad (2.60)$$

The matrix elements are

$$t_{\mathbf{R}_1, \mathbf{R}_2}^{nm} = \int d\mathbf{x} \phi(\mathbf{x})_{n, \mathbf{R}_1}^* \left[-\frac{\hbar^2 \nabla^2}{2m} + \sum_{\mathbf{R}} V(\mathbf{x} - \mathbf{R}) \right] \phi(\mathbf{x})_{m, \mathbf{R}_2}, \quad (2.61)$$

and satisfy

$$t_{\mathbf{R}_1, \mathbf{R}_2}^{nm} = (t_{\mathbf{R}_2, \mathbf{R}_1}^{mn})^*. \quad (2.62)$$

By the property (2.59) it derives that

$$\begin{aligned} t_{\mathbf{R}_1 + \mathbf{R}_0, \mathbf{R}_2 + \mathbf{R}_0}^{nm} &= \int d\mathbf{x} \phi(\mathbf{x})_{n, \mathbf{R}_1 + \mathbf{R}_0}^* \left[-\frac{\hbar^2 \nabla^2}{2m} + \sum_{\mathbf{R}} V(\mathbf{x} - \mathbf{R}) \right] \phi(\mathbf{x})_{m, \mathbf{R}_2 + \mathbf{R}_0} \\ &= \int d\mathbf{x} \phi(\mathbf{x} - \mathbf{R}_0)_{n, \mathbf{R}_1}^* \left[-\frac{\hbar^2 \nabla^2}{2m} + \sum_{\mathbf{R}} V(\mathbf{x} - \mathbf{R}) \right] \phi(\mathbf{x} - \mathbf{R}_0)_{m, \mathbf{R}_2} \\ &= \int d\mathbf{x} \phi(\mathbf{x})_{n, \mathbf{R}_1}^* \left[-\frac{\hbar^2 \nabla^2}{2m} + \sum_{\mathbf{R}} V(\mathbf{x} + \mathbf{R}_0 - \mathbf{R}) \right] \phi(\mathbf{x})_{m, \mathbf{R}_2} = t_{\mathbf{R}_1, \mathbf{R}_2}^{nm}, \end{aligned}$$

since

$$\sum_{\mathbf{R}} V(\mathbf{x} + \mathbf{R}_0 - \mathbf{R}) = \sum_{\mathbf{R}} V(\mathbf{x} - \mathbf{R}).$$

Let us now introduce the operators in the reciprocal lattice through the canonical transformation

$$c_{n, \mathbf{k}, \sigma} = \frac{1}{\sqrt{V}} \sum_{\mathbf{R}} e^{-i\mathbf{k} \cdot \mathbf{R}} c_{n, \mathbf{R}, \sigma}, \quad (2.63)$$

and its inverse

$$c_{n, \mathbf{R}, \sigma} = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{R}} c_{n, \mathbf{k}, \sigma}, \quad (2.64)$$

where V is the number of lattice sites and \mathbf{k} belongs to the reciprocal lattice, namely

$$\sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} = V \delta_{\mathbf{k}0}, \quad \sum_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{R}} = V \delta_{\mathbf{R}0}.$$

One can check that the above transformation is indeed canonical:

$$\begin{aligned} \{c_{n, \mathbf{k}_1, \sigma_1}, c_{m, \mathbf{k}_2, \sigma_2}^\dagger\} &= \frac{1}{V} \sum_{\mathbf{R}_1, \mathbf{R}_2} e^{-i\mathbf{k}_1 \cdot \mathbf{R}_1} e^{i\mathbf{k}_2 \cdot \mathbf{R}_2} \{c_{n, \mathbf{R}_1, \sigma_1}, c_{m, \mathbf{R}_2, \sigma_2}^\dagger\} \\ &= \delta_{nm} \delta_{\sigma_1 \sigma_2} \frac{1}{V} \sum_{\mathbf{R}_1} e^{-i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{R}_1} = \delta_{nm} \delta_{\sigma_1 \sigma_2} \delta_{\mathbf{k}_1 \mathbf{k}_2}. \end{aligned}$$

Let us substitute (2.64) into (2.60):

$$\mathcal{H}_0 = \frac{1}{V} \sum_{\sigma} \sum_{nm} \sum_{\mathbf{R}_1, \mathbf{R}_2} \sum_{\mathbf{k}_1, \mathbf{k}_2} e^{-i\mathbf{k}_1 \cdot \mathbf{R}_1} e^{i\mathbf{k}_2 \cdot \mathbf{R}_2} t_{\mathbf{R}_1, \mathbf{R}_2}^{nm} c_{n, \mathbf{k}_1, \sigma}^\dagger c_{m, \mathbf{k}_2, \sigma}.$$

We notice that

$$\begin{aligned}
& \sum_{\mathbf{R}_1, \mathbf{R}_2} e^{-i\mathbf{k}_1 \cdot \mathbf{R}_1} e^{i\mathbf{k}_2 \cdot \mathbf{R}_2} t_{\mathbf{R}_1, \mathbf{R}_2}^{nm} \\
&= \frac{1}{V} \sum_{\mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_0} e^{-i\mathbf{k}_1 \cdot \mathbf{R}_1} e^{i\mathbf{k}_2 \cdot \mathbf{R}_2} t_{\mathbf{R}_1 - \mathbf{R}_0, \mathbf{R}_2 - \mathbf{R}_0}^{nm} \\
&= \frac{1}{V} \sum_{\mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_0} e^{-i\mathbf{k}_1 \cdot (\mathbf{R}_1 + \mathbf{R}_0)} e^{i\mathbf{k}_2 \cdot (\mathbf{R}_2 + \mathbf{R}_0)} t_{\mathbf{R}_1, \mathbf{R}_2}^{nm} \\
&= \sum_{\mathbf{R}_1, \mathbf{R}_2} e^{-i\mathbf{k}_1 \cdot \mathbf{R}_1} e^{i\mathbf{k}_2 \cdot \mathbf{R}_2} t_{\mathbf{R}_1, \mathbf{R}_2}^{nm} \frac{1}{V} \sum_{\mathbf{R}_0} e^{-i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{R}_0} \\
&= \delta_{\mathbf{k}_1 \mathbf{k}_2} \sum_{\mathbf{R}_1, \mathbf{R}_2} e^{-i\mathbf{k}_1 \cdot (\mathbf{R}_1 - \mathbf{R}_2)} t_{\mathbf{R}_1, \mathbf{R}_2}^{nm} = V \delta_{\mathbf{k}_1 \mathbf{k}_2} t_{\mathbf{k}_1}^{nm},
\end{aligned}$$

where we define

$$t_{\mathbf{k}}^{nm} \equiv \frac{1}{V} \sum_{\mathbf{R}_1, \mathbf{R}_2} e^{-i\mathbf{k} \cdot (\mathbf{R}_1 - \mathbf{R}_2)} t_{\mathbf{R}_1, \mathbf{R}_2}^{nm} = \sum_{\mathbf{R}} e^{-i\mathbf{k} \cdot \mathbf{R}} t_{\mathbf{R}, \mathbf{0}}^{nm}. \quad (2.65)$$

Since (2.62) holds it also follows that

$$\begin{aligned}
(t_{\mathbf{k}}^{nm})^* &= \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} (t_{\mathbf{R}, \mathbf{0}}^{nm})^* \\
&= \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} t_{\mathbf{0}, \mathbf{R}}^{mn} = \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} t_{-\mathbf{R}, \mathbf{0}}^{mn} \\
&= \sum_{\mathbf{R}} e^{-i\mathbf{k} \cdot \mathbf{R}} t_{\mathbf{R}, \mathbf{0}}^{mn} = t_{\mathbf{k}}^{mn},
\end{aligned}$$

namely the matrix $\tilde{t}_{\mathbf{k}}$, with elements $t_{\mathbf{k}}^{mn}$, is hermitean. The Hamiltonian is therefore

$$\mathcal{H}_0 = \sum_{\sigma} \sum_{nm} \sum_{\mathbf{k}} t_{\mathbf{k}}^{nm} c_{n, \mathbf{k}, \sigma}^\dagger c_{m, \mathbf{k}, \sigma}. \quad (2.66)$$

As we said $\tilde{t}_{\mathbf{k}}$ is hermitean, hence it is possible to write

$$\tilde{t}_{\mathbf{k}} = \tilde{U}(\mathbf{k})^\dagger \tilde{\epsilon}_{\mathbf{k}} \tilde{U}(\mathbf{k}) \rightarrow t_{\mathbf{k}}^{nm} = U^\dagger(\mathbf{k})_{ni} \epsilon_{i, \mathbf{k}} U(\mathbf{k})_{im},$$

with $\tilde{U}(\mathbf{k})^\dagger \tilde{U}(\mathbf{k}) = \tilde{I}$. Therefore, upon the canonical transformation

$$c_{i, \mathbf{k}, \sigma} = \sum_n U(\mathbf{k})_{in} c_{n, \mathbf{k}, \sigma},$$

the non interacting Hamiltonian gets a diagonal form

$$\mathcal{H}_0 = \sum_{\sigma} \sum_i \sum_{\mathbf{k}} \epsilon_{i,\mathbf{k}} c_{i,\mathbf{k},\sigma}^{\dagger} c_{i,\mathbf{k},\sigma}. \quad (2.67)$$

The index i identifies the bands, and $\epsilon_{i,\mathbf{k}}$ is the energy dispersion in the reciprocal lattice: we have thus obtained the band structure.

We can formally write

$$c_{i,\mathbf{k},\sigma} = \frac{1}{\sqrt{V}} \sum_{\mathbf{R}} e^{-i\mathbf{R}\cdot\mathbf{k}} c_{i,\mathbf{R},\sigma},$$

thus introducing a new basis of Wannier functions. Since the Fermi field is invariant upon the basis choice, then

$$\begin{aligned} \Psi_{\sigma}(\mathbf{x}) &= \sum_{\mathbf{R},n} \phi(\mathbf{x})_{n,\mathbf{R}} \chi_{\sigma} c_{n,\mathbf{R},\sigma} = \frac{1}{\sqrt{V}} \sum_{\mathbf{R},n,\mathbf{k}} \phi(\mathbf{x})_{n,\mathbf{R}} \chi_{\sigma} e^{i\mathbf{k}\cdot\mathbf{R}} c_{n,\mathbf{k},\sigma} \\ &= \frac{1}{\sqrt{V}} \sum_{\mathbf{R},n,i,\mathbf{k}} \phi(\mathbf{x})_{n,\mathbf{R}} \chi_{\sigma} e^{i\mathbf{k}\cdot\mathbf{R}} U^{\dagger}(\mathbf{k})_{ni} c_{i,\mathbf{k},\sigma} \\ &= \frac{1}{V} \sum_{\mathbf{R},\mathbf{R}',n,i,\mathbf{k}} \phi(\mathbf{x})_{n,\mathbf{R}} \chi_{\sigma} e^{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')} U^{\dagger}(\mathbf{k})_{ni} c_{i,\mathbf{R}',\sigma} \equiv \sum_{\mathbf{R}'} \phi(\mathbf{x})_{i,\mathbf{R}'} \chi_{\sigma} c_{i,\mathbf{R}',\sigma}, \end{aligned}$$

thus implying the following expression of the new Wannier functions

$$\phi(\mathbf{x})_{i,\mathbf{R}'} = \frac{1}{V} \sum_{n,\mathbf{R},\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')} U^{\dagger}(\mathbf{k})_{ni} \phi(\mathbf{x})_{n,\mathbf{R}}. \quad (2.68)$$

Going back to the Hamiltonian in the diagonal basis, we can also rewrite it as

$$\begin{aligned} \hat{H}_0 &= \sum_{\sigma} \sum_i \sum_{\mathbf{k}} \epsilon_{i,\mathbf{k}} c_{i,\mathbf{k},\sigma}^{\dagger} c_{i,\mathbf{k},\sigma} \\ &= \frac{1}{V} \sum_{\sigma} \sum_i \sum_{\mathbf{k}} \sum_{\mathbf{R}_1, \mathbf{R}_2} \epsilon_{i,\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{R}_1-\mathbf{R}_2)} c_{i,\mathbf{R}_1,\sigma}^{\dagger} c_{i,\mathbf{R}_2,\sigma} \\ &\equiv \sum_{\sigma} \sum_i \sum_{\mathbf{R}_1, \mathbf{R}_2} t_{\mathbf{R}_1, \mathbf{R}_2}^i c_{i,\mathbf{R}_1,\sigma}^{\dagger} c_{i,\mathbf{R}_2,\sigma}, \end{aligned} \quad (2.69)$$

namely like a tight-binding Hamiltonian, diagonal in the band index. Once we know the band structure, the ground state of the non interacting Hamiltonian is simply obtained by filling all the lowest bands with the available electrons. If the highest occupied band is full, the model is a band insulator, otherwise is a metal. In particular, since each band can accomodate $2V$ electrons, V of spin up and V of spin down, a necessary condition for a band insulator is to have

an even number of available electrons per unit cell. This is not sufficient since the bands may overlap.

Exercises:

- Calculate the formal expression of the Fourier transform of the density $\rho(\mathbf{q})$ in the basis of eigenoperators of \mathcal{H}_0 , $c_{i,\mathbf{k},\sigma}^\dagger$ and $c_{i,\mathbf{k},\sigma}$;
- Do the same calculation for the current density $\mathbf{J}(\mathbf{x})$, and discuss the meaning of the f -sume rule, Eq. (2.57) in this representation.

2.6.1 Hubbard models

In many physical situations, the Wannier orbitals $\phi(\mathbf{x})_{i,\mathbf{R}}$'s in Eq. (2.68) for the highest occupied bands (valence bands) are quite delocalized, hence the lattice vector label \mathbf{R} loses its physical meaning. In those cases, although formally exact, the tight-binding way (2.69) of rewriting the non interacting Hamiltonian is of little use.³ However there is a wide class of materials, commonly called *strongly correlated systems*, where the tight-binding formalism is meaningful. There the valence bands derive from d or f orbitals of transition metals, rare earth or actinides, and the Wannier orbitals keep noticeable atomic character, thus leading to short range hopping elements $t_{\mathbf{R}_1,\mathbf{R}_2}^i$'s. Let us consider just the above situation and write down the left-over electron-electron interaction in the Wannier basis. We further assume that there is only one valence band well separated from lower and higher ones, so that we are allowed to neglect interband transition processes induced by the interaction. Since we take into account only one band, we are going to drop the band index i , so that the Wannier orbitals for the valence band are $\phi_{\mathbf{R}}(\mathbf{x})$ and the tight-binding term projected on the same band is

$$\hat{H}_0 = \sum_{\sigma} \sum_{\mathbf{R}_1, \mathbf{R}_2} t_{\mathbf{R}_1, \mathbf{R}_2} c_{\mathbf{R}_1 \sigma}^\dagger c_{\mathbf{R}_2 \sigma}. \quad (2.70)$$

The interaction term within the valence band is given by

$$\hat{H}_{int} = \frac{1}{2} \sum_{\sigma_1 \sigma_2} \sum_{\mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_3, \mathbf{R}_4} U_{\mathbf{R}_1, \mathbf{R}_2; \mathbf{R}_3, \mathbf{R}_4} c_{\mathbf{R}_1 \sigma_1}^\dagger c_{\mathbf{R}_2 \sigma_2}^\dagger c_{\mathbf{R}_3 \sigma_2} c_{\mathbf{R}_4 \sigma_1}, \quad (2.71)$$

where

$$U_{\mathbf{R}_1, \mathbf{R}_2; \mathbf{R}_3, \mathbf{R}_4} = \int d\mathbf{x} d\mathbf{y} \phi_{\mathbf{R}_1}(\mathbf{x})^* \phi_{\mathbf{R}_2}(\mathbf{y})^* U(\mathbf{x} - \mathbf{y}) \phi_{\mathbf{R}_3}(\mathbf{y}) \phi_{\mathbf{R}_4}(\mathbf{x}). \quad (2.72)$$

Let us make use of our assumption of well localized Wannier orbitals, namely that $\phi_{\mathbf{R}}(\mathbf{x})$ decays sufficiently fast with $|\mathbf{x} - \mathbf{R}|$. Within this assumption, the leading matrix element is when all lattice sites are the same:

$$U_{\mathbf{R}, \mathbf{R}; \mathbf{R}, \mathbf{R}} \equiv U. \quad (2.73)$$

³For instance the hopping matrix elements $t_{\mathbf{R}_1, \mathbf{R}_2}^i$ turns out to be long ranged.

This term gives rise to an interaction

$$\hat{H}_U = \frac{U}{2} \sum_{\mathbf{R}} n_{\mathbf{R}} n_{\mathbf{R}}, \quad (2.74)$$

where the operator

$$n_{\mathbf{R}} = \sum_{\sigma} c_{\mathbf{R}\sigma}^{\dagger} c_{\mathbf{R}\sigma},$$

counts the number of particles at site \mathbf{R} . The interaction term (2.74), which simply describes an on-site Coulomb repulsion, plus the hopping (2.70) represent the so-called *Hubbard model*, which is the prototype of the strongly-correlated lattice models.

Let us continue and consider in (2.72) two other cases: either (1) $\mathbf{R}_1 = \mathbf{R}_4$, $\mathbf{R}_2 = \mathbf{R}_3$ with \mathbf{R}_2 nearest neighbor of \mathbf{R}_1 or (2) $\mathbf{R}_1 = \mathbf{R}_3$, $\mathbf{R}_2 = \mathbf{R}_4$ still with \mathbf{R}_2 nearest neighbor of \mathbf{R}_1 . In case (1) we obtain

$$\frac{U_1}{2} \sum_{<\mathbf{R}\mathbf{R}'>} n_{\mathbf{R}} n_{\mathbf{R}'},$$

where $<\mathbf{R}\mathbf{R}'>$ stands for nearest neighbor sites and

$$U_1 = U_{\mathbf{R},\mathbf{R}';\mathbf{R}',\mathbf{R}}.$$

In case (2) we find

$$\frac{U_2}{2} \sum_{<\mathbf{R}\mathbf{R}'>} \sum_{\sigma\sigma'} c_{\mathbf{R}\sigma}^{\dagger} c_{\mathbf{R}'\sigma'}^{\dagger} c_{\mathbf{R}\sigma'} c_{\mathbf{R}'\sigma} = -\frac{U_2}{2} \sum_{<\mathbf{R}\mathbf{R}'>} \sum_{\sigma\sigma'} c_{\mathbf{R}\sigma}^{\dagger} c_{\mathbf{R}\sigma'}^{\dagger} c_{\mathbf{R}'\sigma'}^{\dagger} c_{\mathbf{R}'\sigma},$$

where

$$U_2 = U_{\mathbf{R},\mathbf{R}';\mathbf{R},\mathbf{R}'}.$$

One can easily show that

$$\sum_{\sigma\sigma'} c_{\mathbf{R}\sigma}^{\dagger} c_{\mathbf{R}\sigma'}^{\dagger} c_{\mathbf{R}'\sigma'}^{\dagger} c_{\mathbf{R}'\sigma} = \frac{1}{2} [n_{\mathbf{R}} n_{\mathbf{R}'} + 4\mathbf{S}_{\mathbf{R}} \cdot \mathbf{S}_{\mathbf{R}'}], \quad (2.75)$$

where the spin density operator

$$\mathbf{S}_{\mathbf{R}} = \frac{1}{2} \sum_{\alpha\beta} c_{\mathbf{R}\alpha}^{\dagger} \sigma_{\alpha\beta} c_{\mathbf{R}\beta},$$

being $\sigma = (\sigma_1, \sigma_2, \sigma_3)$, with σ_i 's the Pauli matrices. Therefore, upon defining $V = U_1 - U_2/2$ and $J_{ex} = -2U_2$, the whole nearest neighbor interaction reads

$$\hat{H}_{n.n.} = \frac{V}{2} \sum_{<\mathbf{R}\mathbf{R}'>} n_{\mathbf{R}} n_{\mathbf{R}'} + \frac{J_{ex}}{2} \sum_{<\mathbf{R}\mathbf{R}'>} \mathbf{S}_{\mathbf{R}} \cdot \mathbf{S}_{\mathbf{R}'}. \quad (2.76)$$

Since $U_1 > U_2 > 0$, the first term describes a nearest-neighbor repulsion, while the second a spin exchange which tends to aligns the spin ferromagnetically since $J < 0$, so called *direct exchange*. Therefore, although we have started from a spin independent interaction, in the Wannier basis we have been able to identify a spin interaction, thus showing in a simple way how magnetism emerges out of the Coulomb repulsion.

2.6.2 The Mott insulator within the Hubbard model

Let us summarize the approximate Hubbard Hamiltonian which we have so far derived, by further assuming a nearest neighbor hopping:

$$\begin{aligned}\hat{H} &= -t \sum_{\sigma} \sum_{\langle \mathbf{R} \mathbf{R}' \rangle} c_{\mathbf{R} \sigma}^{\dagger} c_{\mathbf{R}' \sigma} + \frac{U}{2} \sum_{\mathbf{R}} n_{\mathbf{R}} n_{\mathbf{R}} + \frac{V}{2} \sum_{\langle \mathbf{R} \mathbf{R}' \rangle} n_{\mathbf{R}} n_{\mathbf{R}'} + \frac{J_{ex}}{2} \sum_{\langle \mathbf{R} \mathbf{R}' \rangle} \mathbf{S}_{\mathbf{R}} \cdot \mathbf{S}_{\mathbf{R}'} \\ &= \hat{H}_0 + \hat{H}_{int}.\end{aligned}$$

By construction $U > V > 0$ and $J_{ex} < 0$. We consider the case in which the number of valence electrons is equal to the number of sites N . In the absence of interaction, the hopping forms a band which can accommodate $2N$ electrons: therefore the band is half-filled and the system is metallic.

Exercise: Consider the nearest neighbor tight-binding model

$$\mathcal{H} = -t \sum_{\sigma} \sum_{\langle \mathbf{R} \mathbf{R}' \rangle} c_{\mathbf{R} \sigma}^{\dagger} c_{\mathbf{R}' \sigma},$$

with $t > 0$ in a two-dimensional square lattice. The number of electrons is equal to the number of sites. Find the shape of the Fermi surface.

Let us analyse the opposite case of a very large $U \gg t, V, |J_{ex}|$. In this case we should start from the configuration which minimizes the Coulomb repulsion U and treat what is left by perturbation theory. This lowest energy electronic configuration is the one in which each site is singly occupied. Indeed the energy cost in having just an empty site and a doubly occupied one instead of two singly occupied sites is given by

$$E(2) + E(0) - 2E(1) = 2U + 0 - 2\frac{U}{2} = U,$$

and is much larger then the energy gain in letting the electrons move, which is of order t . In this situation the model describes an insulator, but of a particular kind. Namely the insulating state is driven by the strong correlation, while the conventional band structure argument would predict always a metal. This correlation-induced insulator is called a *Mott insulator*. Therefore, as the strength of U increases with respect to the bandwidth proportional to t , an interaction

driven metal-to-insulator transition, commonly referred as a *Mott transition*, should occur at a critical U_c . However, the configuration with one electron per site is hugely degenerate, since the electron can have either spin up or down. There are 2^N degenerate states with one electron per site, which are going to be split by the left-over terms in the Hamiltonian. The nearest neighbor interaction V is not effective in splitting the degeneracy. On the contrary, the direct exchange does play a role and tends to prefer the configuration in which all spins are aligned – a ferromagnetic ordering. Yet, this is not the only source of spin correlations. Indeed also the hopping term is able to split the degeneracy within second order in perturbation theory. Let us focus on two states which only differs in the spin configurations of two nearest neighbor sites: $|\sigma_{\mathbf{R}_1}, \sigma_{\mathbf{R}_2}\rangle$ and $|\sigma'_{\mathbf{R}_1}, \sigma'_{\mathbf{R}_2}\rangle$. Within second order in t we obtain a matrix element between these two states given by

$$t^2 \sum_n \sum_{\sigma\sigma'} \langle \sigma_{\mathbf{R}_1}, \sigma_{\mathbf{R}_2} | \left(c_{\mathbf{R}_1\sigma}^\dagger c_{\mathbf{R}_2\sigma} + H.c. \right) |n\rangle \frac{1}{E_0 - E_n} \langle n | \left(c_{\mathbf{R}_1\sigma'}^\dagger c_{\mathbf{R}_2\sigma'} + H.c. \right) |\sigma'_{\mathbf{R}_1}, \sigma'_{\mathbf{R}_2}\rangle,$$

where $E_0 = NU/2$ is the energy of the degenerate ground states with all singly occupied sites, and $|n\rangle$ an excited state with energy E_n . Since the hopping creates one empty and one doubly occupied site out of two singly occupied ones, $E_0 - E_n = -U$. Moreover the sum over the intermediate states act as a complete sum, so that we can write also

$$-\frac{t^2}{U} \sum_{\sigma\sigma'} \langle \sigma_{\mathbf{R}_1}, \sigma_{\mathbf{R}_2} | \left(c_{\mathbf{R}_1\sigma}^\dagger c_{\mathbf{R}_2\sigma} c_{\mathbf{R}_2\sigma'}^\dagger c_{\mathbf{R}_1\sigma'} + c_{\mathbf{R}_2\sigma}^\dagger c_{\mathbf{R}_1\sigma} c_{\mathbf{R}_1\sigma'}^\dagger c_{\mathbf{R}_2\sigma'} \right) |\sigma'_{\mathbf{R}_1}, \sigma'_{\mathbf{R}_2}\rangle.$$

By means of (2.75) we therefore find that the operator responsible of the additional splitting is

$$\begin{aligned} & -\frac{t^2}{U} \sum_{\sigma\sigma'} \left(c_{\mathbf{R}_1\sigma}^\dagger c_{\mathbf{R}_2\sigma} c_{\mathbf{R}_2\sigma'}^\dagger c_{\mathbf{R}_1\sigma'} + c_{\mathbf{R}_2\sigma}^\dagger c_{\mathbf{R}_1\sigma} c_{\mathbf{R}_1\sigma'}^\dagger c_{\mathbf{R}_2\sigma'} \right) \\ &= \frac{t^2}{U} \sum_{\sigma\sigma'} 2 c_{\mathbf{R}_1\sigma}^\dagger c_{\mathbf{R}_1\sigma'} c_{\mathbf{R}_2\sigma'}^\dagger c_{\mathbf{R}_2\sigma} - (n_{\mathbf{R}_1\sigma} + n_{\mathbf{R}_2\sigma}) \delta_{\sigma\sigma'} \\ &= \frac{4t^2}{U} \left[\mathbf{S}_{\mathbf{R}_1} \cdot \mathbf{S}_{\mathbf{R}_2} + \frac{1}{4} (n_{\mathbf{R}_1} n_{\mathbf{R}_2} - n_{\mathbf{R}_1} - n_{\mathbf{R}_2}) \right]. \end{aligned}$$

Since the last term is a constant over states where each site is singly occupied, the relevant part is just

$$\frac{2t^2}{U} \sum_{\langle \mathbf{R}\mathbf{R}' \rangle} \mathbf{S}_{\mathbf{R}} \cdot \mathbf{S}_{\mathbf{R}'}, \quad (2.77)$$

the missing factor two coming from the fact that in the sum over nearest neighbors each bond is counted twice. Therefore the second order perturbation theory in the hopping gives rise to a novel spin exchange which is antiferromagnetic, usually called *super-exchange*. All together, the

large U effective Hamiltonian describes localized spin-1/2's (each site occupied by one electron) coupled by the spin exchange

$$\hat{H}_{Heis} = \frac{J}{2} \sum_{\langle \mathbf{R}\mathbf{R}' \rangle} \mathbf{S}_{\mathbf{R}} \cdot \mathbf{S}_{\mathbf{R}'}, \quad (2.78)$$

where

$$J = J_{ex} + \frac{4t^2}{U} = -2U_2 + \frac{4t^2}{U}.$$

The spin exchange may be either ferromagnetic or antiferromagnetic depending on the strength of the direct- with respect to the super-exchange couplings. The effective Hamiltonian (2.78) describes an *Heisenberg model*.

2.7 Spin wave theory in the Heisenberg model

We have previously shown how magnetism may emerge in a single band Mott insulator where strong Coulomb repulsion localizes the electrons which become effectively local moments. We have also shown that both the Coulomb repulsion itself, via the direct exchange, and the covalent binding, via the super-exchange proportional to the square of the hopping, induce a coupling among the local moments which has the form

$$\hat{H}_{Heis} = \sum_{\mathbf{R}, \mathbf{R}'} J_{\mathbf{R}, \mathbf{R}'} \mathbf{S}_{\mathbf{R}} \cdot \mathbf{S}_{\mathbf{R}'}. \quad (2.79)$$

Notice that, by lattice translational symmetry,

$$J_{\mathbf{R}, \mathbf{R}'} = J_{\mathbf{R}', \mathbf{R}} = J_{\mathbf{R}' - \mathbf{R} - \mathbf{R}', \mathbf{R} - \mathbf{R} - \mathbf{R}'} = J_{-\mathbf{R}, -\mathbf{R}'},$$

namely the exchange is inversion symmetric. In the single band case we discussed, the spins have magnitude $S = 1/2$, but, in what follows, we will consider the general case of arbitrary S . As a result, the Mott insulator will likely be magnetically ordered according to the properties of the exchange terms. If the spins were classical vectors, then the classical ground state would show a magnetic order of the form

$$\langle \mathbf{S}_{\mathbf{R}} \rangle = S [\mathbf{u} \cos(\mathbf{Q} \cdot \mathbf{R}) + \mathbf{v} \sin(\mathbf{Q} \cdot \mathbf{R})], \quad (2.80)$$

with \mathbf{u} and \mathbf{v} two orthogonal unit vectors. Upon inserting this expression into (2.79), we find a classical energy

$$E(\mathbf{Q}) = \sum_{\mathbf{R}, \mathbf{R}'} J_{\mathbf{R}, \mathbf{R}'} \cos(\mathbf{Q} \cdot (\mathbf{R} - \mathbf{R}')) = N \sum_{\mathbf{R}} J_{\mathbf{R}, \mathbf{0}} \cos(\mathbf{Q} \cdot \mathbf{R}) = \frac{N}{2} (J_{\mathbf{Q}} + J_{-\mathbf{Q}}) = NJ_{\mathbf{Q}},^4$$

⁴Since, as we showed, the exchange is inversion symmetric, namely $J_{\mathbf{R}, \mathbf{0}} = J_{-\mathbf{R}, \mathbf{0}}$, then $J_{\mathbf{Q}} = J_{\mathbf{Q}}^* = J_{-\mathbf{Q}}$

which is minimized by the value of \mathbf{Q} for which the $J_{\mathbf{Q}}$ is minimum. The classical ground state energy does not depend on \mathbf{u} and \mathbf{v} , reflecting the global spin-rotational symmetry. In the reciprocal lattice, (2.80) implies an order parameter

$$\langle \mathbf{S}_{\mathbf{q}} \rangle = \sum_{\mathbf{R}} e^{-i\mathbf{q} \cdot \mathbf{R}} \langle \mathbf{S}_{\mathbf{R}} \rangle = \frac{SN}{2} (\mathbf{u} - i\mathbf{v}) \delta_{\mathbf{q}, \mathbf{Q}} + \frac{SN}{2} (\mathbf{u} + i\mathbf{v}) \delta_{\mathbf{q}, -\mathbf{Q}}. \quad (2.81)$$

In reality the spins are quantum operators satisfying the usual commutation relations

$$[S_{\mathbf{R}}^a, S_{\mathbf{R}'}^b] = i\epsilon_{abc} S_{\mathbf{R}}^c \delta_{\mathbf{R}\mathbf{R}'},$$

which, in the reciprocal lattice, transform into

$$[S_{\mathbf{q}}^a, S_{\mathbf{q}'}^b] = i\epsilon_{abc} S_{\mathbf{q}+\mathbf{q}'}^c.$$

Therefore, through the Heisenberg equation of motion

$$i\hbar \frac{d\mathbf{S}_{\mathbf{R}}}{dt} = [\mathbf{S}_{\mathbf{R}}, \hat{H}_{Heis}] = -i \sum_{\mathbf{R}'} J_{\mathbf{R}, \mathbf{R}'} \mathbf{S}_{\mathbf{R}} \times \mathbf{S}_{\mathbf{R}'},$$

we find that

$$i\hbar \frac{d\mathbf{S}_{\mathbf{Q}}}{dt} = -i \sum_{\mathbf{q}} \frac{J_{\mathbf{q}}}{N} \mathbf{S}_{\mathbf{q}+\mathbf{Q}} \times \mathbf{S}_{-\mathbf{q}}.$$

Since the right hand side is non zero, then the classical order parameter does not correspond quantum mechanically to a conserved quantity. It turns this implies that quantum fluctuations are going to reduce the magnitude of the classical order parameter. There is just one exception when the classical ordering wave-vector $\mathbf{Q} = \mathbf{0}$, which corresponds to a ferromagnetic order. In this case the order parameter is just the total magnetization, which is indeed a conserved quantity. Therefore, if all J 's are negative so that the $\min(J_{\mathbf{q}})$ is at $\mathbf{Q} = \mathbf{0}$, the quantum ground state remains the classical fully polarized ferromagnet. In all other cases when $\mathbf{Q} \neq \mathbf{0}$, we do not know *a priori* if the classical ordered phase is going to survive quantum fluctuations. A quite simple but effective way to analyse the role of quantum fluctuations is by the so-called *spin-wave theory*.

We now show how this method works for the simple example of an antiferromagnetic Heisenberg model with nearest neighbor exchange on an hypercubic lattice. The Hamiltonian is given by

$$\hat{H}_{Heis} = J \sum_{\langle \mathbf{R} \mathbf{R}' \rangle} \mathbf{S}_{\mathbf{R}} \cdot \mathbf{S}_{\mathbf{R}'}, \quad (2.82)$$

with $J > 0$. The classical ground state is the Néel antiferromagnet with order parameter (we choose to break the SU(2) symmetry along the z -axis)

$$\langle S_{\mathbf{R}}^z \rangle = S \cos(\mathbf{Q} \cdot \mathbf{R}) = S (-1)^R,$$

where $\mathbf{Q} = \pi(1, 1, 1, \dots, 1)$ ⁵ and, if $\mathbf{R} = (n_1, n_2, \dots, n_d)$ with d the dimension of the space, then $R = \sum_{i=1}^d n_i$. Let us go back to the commutation relation

$$[S_{\mathbf{q}}^a, S_{\mathbf{q}'}^b] = i\epsilon_{abc} S_{\mathbf{q}+\mathbf{q}'}^c,$$

and assume that the left hand side is substituted by the classical average value, i.e.

$$[S_{\mathbf{q}}^a, S_{\mathbf{q}'}^b] = i\epsilon_{abz} NS\delta_{\mathbf{Q},\mathbf{q}+\mathbf{q}'},$$

The meaning of this approximation is the following. If we want to analyse the role of quantum fluctuations, we need to study the dynamics of the spin operators which, by the equations of motion, is related to commutators. If the true ground state is a slight modification of the classical one, which has to be checked *a posteriori*, then the commutators can be approximated with their classical averages. Within this approximation

$$[S_{\mathbf{q}}^x, S_{-\mathbf{q}+\mathbf{Q}}^y] \simeq iNS.$$

Yet we have to further impose that

$$\begin{aligned} [S_{\mathbf{q}}^x, S_{\mathbf{Q}}^z] &= -iS_{\mathbf{q}+\mathbf{Q}}^y, \\ [S_{\mathbf{q}}^y, S_{\mathbf{Q}}^z] &= iS_{\mathbf{q}+\mathbf{Q}}^x, \end{aligned}$$

Both conditions can be fulfilled if we write

$$\begin{aligned} S_{\mathbf{q}}^x &= \sqrt{\frac{SN}{2}} (d_{\mathbf{q}} + d_{-\mathbf{q}}^\dagger), \\ S_{\mathbf{q}}^y &= -i\sqrt{\frac{SN}{2}} (d_{\mathbf{q}-\mathbf{Q}} - d_{-\mathbf{q}+\mathbf{Q}}^\dagger), \\ S_{\mathbf{Q}}^z &= SN - \sum_{\mathbf{q}} d_{\mathbf{q}}^\dagger d_{\mathbf{q}}. \end{aligned} \tag{2.83}$$

The operators $d_{\mathbf{q}}$'s and $d_{\mathbf{q}}^\dagger$'s are bosonic and satisfy

$$[d_{\mathbf{q}}, d_{\mathbf{q}'}^\dagger] = \delta_{\mathbf{q},\mathbf{q}'}, \quad [d_{\mathbf{q}}, d_{\mathbf{q}'}] = 0.$$

The expression for the order parameter operator $S_{\mathbf{Q}}^z$ clarifies also the meaning of our starting assumption of a quantum ground state slightly different from the classical one. Indeed this approximation holds if

$$\langle S_{\mathbf{Q}}^z \rangle \sim SN,$$

⁵Notice that $\mathbf{Q} = -\mathbf{Q}$, being the two connected by a reciprocal lattice vector

namely if

$$\frac{1}{N} \sum_{\mathbf{q}} \langle d_{\mathbf{q}}^\dagger d_{\mathbf{q}} \rangle \ll S.$$

Therefore the larger is the spin magnitude S the more correct is the approximation, i.e. the weaker are the effects of quantum fluctuations. The Hamiltonian in the reciprocal lattice is

$$\hat{H}_{Heis} = \frac{1}{N} \sum_{\mathbf{q}} J(\mathbf{q}) \mathbf{S}_{\mathbf{q}} \cdot \mathbf{S}_{-\mathbf{q}},$$

where

$$J(\mathbf{q}) = 2J \sum_{i=1}^d \cos(q_i) \equiv 2J \gamma_{\mathbf{q}},$$

d being the dimension of the space and $\mathbf{q} = (q_1, q_2, \dots, q_d)$. Notice that

$$J(\mathbf{Q}) = -2Jd.$$

Since

$$J(\mathbf{q} + \mathbf{Q}) = 2J \sum_{i=1}^d \cos(q_i + \pi) = -J(\mathbf{q}),$$

we can also rewrite the Hamiltonian, compatibly with our assumption of weak quantum fluctuations, as

$$\begin{aligned} \hat{H}_{Heis} &= \frac{1}{2N} \sum_{\mathbf{q}} J(\mathbf{q}) (\mathbf{S}_{\mathbf{q}} \cdot \mathbf{S}_{-\mathbf{q}} - \mathbf{S}_{\mathbf{q}+\mathbf{Q}} \cdot \mathbf{S}_{-\mathbf{q}+\mathbf{Q}}) \\ &\simeq \frac{1}{2N} \sum_{\mathbf{q}} J(\mathbf{q}) (S_{\mathbf{q}}^x S_{-\mathbf{q}}^x + S_{\mathbf{q}}^y S_{-\mathbf{q}}^y - S_{\mathbf{q}+\mathbf{Q}}^x S_{-\mathbf{q}+\mathbf{Q}}^x - S_{\mathbf{q}+\mathbf{Q}}^y S_{-\mathbf{q}+\mathbf{Q}}^y) \\ &\quad + \frac{1}{N} J(\mathbf{Q}) S_{\mathbf{Q}}^z S_{-\mathbf{Q}}^z, \end{aligned} \tag{2.84}$$

At this stage we should substitute (2.83) into (2.84), keep only bilinear terms and diagonalize the Hamiltonian by a canonical transformation. However it is much better to follow an equivalent route where calculations are simpler. We introduce conjugate variables through

$$x_{\mathbf{q}} = \sqrt{\frac{1}{2}} (d_{\mathbf{q}} + d_{-\mathbf{q}}^\dagger), \tag{2.85}$$

$$p_{\mathbf{q}} = i \sqrt{\frac{1}{2}} (d_{-\mathbf{q}}^\dagger - d_{\mathbf{q}}), \tag{2.86}$$

which satisfy the canonical commutation relation

$$[x_{\mathbf{q}}, p_{\mathbf{q}'}] = i\delta_{\mathbf{q}, -\mathbf{q}'}.$$

In terms of these variables the expressions for the spin operators read

$$\begin{aligned} S_{\mathbf{q}}^x &= \sqrt{SN} x_{\mathbf{q}}, \\ S_{\mathbf{q}}^y &= \sqrt{SN} p_{\mathbf{q}-\mathbf{Q}}, \\ S_{\mathbf{Q}}^z &= \left(S + \frac{1}{2} \right) N - \frac{1}{2} \sum_{\mathbf{q}} x_{\mathbf{q}} x_{-\mathbf{q}} + p_{\mathbf{q}} p_{-\mathbf{q}}, \end{aligned}$$

which substituted into (2.84) and keeping up to order S terms, lead to

$$\begin{aligned} \hat{H}_{Heis} &= \frac{S}{2} \sum_{\mathbf{q}} J(\mathbf{q}) (x_{\mathbf{q}} x_{-\mathbf{q}} + p_{\mathbf{q}-\mathbf{Q}} p_{-\mathbf{q}+\mathbf{Q}} - x_{\mathbf{q}-\mathbf{Q}} x_{-\mathbf{q}+\mathbf{Q}} - p_{\mathbf{q}} p_{-\mathbf{q}}) \\ &\quad + \frac{1}{N} J(\mathbf{Q}) \left(S^2 N^2 + SN^2 - SN \sum_{\mathbf{q}} x_{\mathbf{q}} x_{-\mathbf{q}} + p_{\mathbf{q}} p_{-\mathbf{q}} \right) \\ &= N J(\mathbf{Q}) S (S+1) + S \sum_{\mathbf{q}} J(\mathbf{q}) (x_{\mathbf{q}} x_{-\mathbf{q}} - p_{\mathbf{q}} p_{-\mathbf{q}}) \\ &\quad - S J(\mathbf{Q}) \sum_{\mathbf{q}} (x_{\mathbf{q}} x_{-\mathbf{q}} + p_{\mathbf{q}} p_{-\mathbf{q}}) \\ &= N J(\mathbf{Q}) S (S+1) \\ &\quad + S \sum_{\mathbf{q}} (J(\mathbf{q}) - J(\mathbf{Q})) x_{\mathbf{q}} x_{-\mathbf{q}} + (-J(\mathbf{q}) - J(\mathbf{Q})) p_{\mathbf{q}} p_{-\mathbf{q}}. \end{aligned} \quad (2.87)$$

The constant term $N J(\mathbf{Q}) S^2$ represents the classical Ne  l energy, the rest being the correction due to quantum mechanics. In order to diagonalize this Hamiltonian, let us consider the following canonical transformation

$$x_{\mathbf{q}} = \sqrt{K_{\mathbf{q}}} X_{\mathbf{q}}, \quad (2.88)$$

$$p_{\mathbf{q}} = \sqrt{\frac{1}{K_{\mathbf{q}}}} P_{\mathbf{q}}, \quad (2.89)$$

which preserves the commutation relations provided $K_{\mathbf{q}} = K_{-\mathbf{q}}$. Upon substitution, the quantum fluctuation term transforms into

$$\begin{aligned} &S \sum_{\mathbf{q}} (J(\mathbf{q}) - J(\mathbf{Q})) x_{\mathbf{q}} x_{-\mathbf{q}} + (-J(\mathbf{q}) - J(\mathbf{Q})) p_{\mathbf{q}} p_{-\mathbf{q}} \rightarrow \\ &\rightarrow S \sum_{\mathbf{q}} K_{\mathbf{q}} (J(\mathbf{q}) - J(\mathbf{Q})) X_{\mathbf{q}} X_{-\mathbf{q}} + K_{\mathbf{q}}^{-1} (-J(\mathbf{q}) - J(\mathbf{Q})) P_{\mathbf{q}} P_{-\mathbf{q}}. \end{aligned}$$

If we impose that

$$K_{\mathbf{q}}^2 = \frac{-J(\mathbf{Q}) - J(\mathbf{q})}{-J(\mathbf{Q}) + J(\mathbf{q})}, \quad (2.90)$$

the Hamiltonian becomes that of independent harmonic oscillators, i.e.

$$\hat{H}_{Heis} = N J(\mathbf{Q}) S(S+1) + \frac{1}{2} \sum_{\mathbf{q}} \omega_{\mathbf{q}} (X_{\mathbf{q}} X_{-\mathbf{q}} + P_{\mathbf{q}} P_{-\mathbf{q}}), \quad (2.91)$$

with the dispersion relation defined through

$$\omega_{\mathbf{q}} = 2S \sqrt{(-J(\mathbf{Q}) - J(\mathbf{q})) (-J(\mathbf{Q}) + J(\mathbf{q}))} = 4S J \sqrt{(d - \gamma_{\mathbf{q}})(d + \gamma_{\mathbf{q}})}. \quad (2.92)$$

Notice that, since $d \geq |\gamma_{\mathbf{q}}|$, the frequencies are positive real numbers. It is clear that the Hamiltonian has a diagonal form. Indeed if we introduce new bosonic operators through

$$\begin{aligned} X_{\mathbf{q}} &= \sqrt{\frac{1}{2}} (b_{\mathbf{q}} + b_{-\mathbf{q}}^{\dagger}), \\ P_{\mathbf{q}} &= -i \sqrt{\frac{1}{2}} (b_{\mathbf{q}} - b_{-\mathbf{q}}^{\dagger}), \end{aligned}$$

the Hamiltonian transforms into

$$\hat{H}_{Heis} = N J(\mathbf{Q}) S(S+1) + \sum_{\mathbf{q}} \omega_{\mathbf{q}} \left(b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} + \frac{1}{2} \right), \quad (2.93)$$

thus showing that the eigenstates are Fock states in the b -basis $|\{n_{\mathbf{q}}\}\rangle$ with energies

$$\hat{H}_{Heis} |\{n_{\mathbf{q}}\}\rangle = \left[N J(\mathbf{Q}) S(S+1) + \sum_{\mathbf{q}} \omega_{\mathbf{q}} \left(n_{\mathbf{q}} + \frac{1}{2} \right) \right] |\{n_{\mathbf{q}}\}\rangle \equiv E[\{n_{\mathbf{q}}\}] |\{n_{\mathbf{q}}\}\rangle.$$

The elementary bosonic excitations are called **spin-waves**. The vacuum is the ground state, whose energy per site including quantum fluctuations is

$$\begin{aligned} E_0 &= -2JdS^2 - \frac{1}{N} \sum_{\mathbf{q}} \left(2SJd - \frac{1}{2} \omega_{\mathbf{q}} \right) \\ &= E_{class} - \frac{2JS}{N} \sum_{\mathbf{q}} \left[d - \sqrt{(d - \gamma_{\mathbf{q}})(d + \gamma_{\mathbf{q}})} \right] < E_{class}, \end{aligned}$$

which, as expected, is lower than the classical counterpart E_{class} .

Let us analyse the energy spectrum of the spin-waves. First we notice that

$$\gamma_{\mathbf{q}} = -\gamma_{\mathbf{q}-\mathbf{Q}},$$

hence that $\omega_{\mathbf{q}} = \omega_{\mathbf{q}+\mathbf{Q}}$, showing that the true Brillouin zone is half of the original one. This is because the Néel state breaks translational symmetry and the new unit cell contains two sites. Secondly, by expanding (2.92) close to $\mathbf{q} = 0$, which as we said is equivalent to $\mathbf{q} = \mathbf{Q}$, and since

$$\gamma_{\mathbf{q}} \simeq d - \frac{1}{2}\mathbf{q} \cdot \mathbf{q},$$

we find that

$$\omega_{\mathbf{q}} = 4S J \sqrt{(d - \gamma_{\mathbf{q}})(d + \gamma_{\mathbf{q}})} \simeq 4S J \sqrt{d} |\mathbf{q}| \equiv v |\mathbf{q}|,$$

namely a linearly vanishing dispersion with velocity $v = 4S J \sqrt{d}$. This was actually predictable by the Goldstone theorem which states that when a continuous symmetry is broken, in our case the spin SU(2), and in the absence of long range interaction, there should exist a mode, the Goldstone mode, with vanishing energy as $\mathbf{q} \rightarrow \mathbf{0}$.

Let us go back to the canonical transformation (2.88) and (2.89). One can prove that this transformation is accomplished by the unitary operator

$$\hat{U} = \exp \left[-\frac{i}{2} \sum_{\mathbf{q}} \ln K_{\mathbf{q}} x_{\mathbf{q}} p_{-\mathbf{q}} \right], \quad (2.94)$$

namely that

$$\hat{U}^\dagger x_{\mathbf{q}} \hat{U} = \sqrt{K_{\mathbf{q}}} x_{\mathbf{q}}. \quad (2.95)$$

This result can be obtained through to the following expression

$$e^{-A} B e^A = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} C_n,$$

where $C_0 = B$ and $C_n = [A, C_{n-1}]$.

Exercise: Prove the above statement, namely that (2.94) gives rise to (2.95).

Therefore the unitary transformation (2.94) applied to the Hamiltonian (2.87) gives

$$\hat{U}^\dagger \hat{H}_{Heis} \hat{U} = E_0 + \frac{1}{2} \sum_{\mathbf{q}} \omega_{\mathbf{q}} (x_{\mathbf{q}} x_{-\mathbf{q}} + p_{\mathbf{q}} p_{-\mathbf{q}} - 1),$$

namely the desired diagonal form. This way of rewriting the canonical transformation is quite useful since it allows to identify the eigenstates in a simple way. Let us consider the state

$$|\{\{n_{\mathbf{q}}\}\}\rangle = \hat{U} |\{\{n_{\mathbf{q}}\}\}\rangle_0,$$

where $|\{\{n_{\mathbf{q}}\}\}\rangle_0$ is a Fock state in the old basis with the occupation number configuration $\{n_{\mathbf{q}}\}$. Then

$$\hat{H}_{Heis} |\{\{n_{\mathbf{q}}\}\}\rangle = \hat{H}_{Heis} \hat{U} |\{\{n_{\mathbf{q}}\}\}\rangle_0$$

$$\begin{aligned}
&= \hat{U} \hat{U}^\dagger \hat{H}_{Heis} \hat{U} |\{\mathbf{n}_q\}\rangle_0 = \hat{U} \left[E_0 + \sum_{\mathbf{q}} \omega_{\mathbf{q}} \hat{n}_{\mathbf{q}} \right] |\{\mathbf{n}_q\}\rangle_0 \\
&= \left[E_0 + \sum_{\mathbf{q}} \omega_{\mathbf{q}} n_{\mathbf{q}} \right] \hat{U} |\{\mathbf{n}_q\}\rangle_0 = E[\{\mathbf{n}_q\}] |\{\mathbf{n}_q\}\rangle,
\end{aligned}$$

namely it is an eigenstate with energy

$$E[\{\mathbf{n}_q\}] = \left[E_0 + \sum_{\mathbf{q}} \omega_{\mathbf{q}} n_{\mathbf{q}} \right].$$

Analogously, the new vacuum state can be obtained by the old one through

$$|0\rangle = \hat{U} |0\rangle_0.$$

Finally we have to check whether our approximation is valid. Let us evaluate the ground state average value of the order parameter

$$\begin{aligned}
M &= \frac{1}{N} \langle 0 | \hat{S}_{\mathbf{Q}}^z | 0 \rangle = S + \frac{1}{2} - \frac{1}{2N} \sum_{\mathbf{q}} \langle 0 | x_{\mathbf{q}} x_{-\mathbf{q}} + p_{\mathbf{q}} p_{-\mathbf{q}} | 0 \rangle \\
&= S + \frac{1}{2} - \frac{1}{2N} \sum_{\mathbf{q}} \langle 0 | K_{\mathbf{q}} X_{\mathbf{q}} X_{-\mathbf{q}} + K_{\mathbf{q}}^{-1} P_{\mathbf{q}} P_{-\mathbf{q}} | 0 \rangle \\
&= S + \frac{1}{2} - \frac{1}{4N} \sum_{\mathbf{q}} K_{\mathbf{q}} + K_{\mathbf{q}}^{-1} \\
&= S + \frac{1}{2} - \frac{1}{2N} \sum_{\mathbf{q}} \sqrt{\frac{d + \gamma_{\mathbf{q}}}{d - \gamma_{\mathbf{q}}}}, \tag{2.96}
\end{aligned}$$

where we used the fact that on the new vacuum

$$\langle 0 | X_{\mathbf{q}} X_{-\mathbf{q}} | 0 \rangle = \langle 0 | P_{\mathbf{q}} P_{-\mathbf{q}} | 0 \rangle = \frac{1}{2},$$

and that $K_{\mathbf{q}}^{-1} = K_{\mathbf{q}+\mathbf{Q}}$. If $S - M \ll 1$ then the approximation indeed holds. The only dangerous region in the sum is when $d \sim \gamma_{\mathbf{q}}$, i.e. when the spin-wave energy vanishes. Here the sum behaves as

$$\frac{1}{2N} \sum_{\mathbf{q}} \sqrt{\frac{d + \gamma_{\mathbf{q}}}{d - \gamma_{\mathbf{q}}}} \sim \int \frac{d\mathbf{q}}{|\mathbf{q}|}.$$

This integral is convergent for $d \geq 2$, but is singular in one dimension. Therefore the spin wave approximation is always wrong in one dimension, in agreement with Mermin-Wagner theorem

which states that a continuous symmetry can not be broken in 1+1 dimensions (A quantum problem in d dimensions corresponds to a classical one in $d + 1$).

To complete our analysis, let us evaluate the contribution of thermal fluctuations, namely let us move to finite temperature T . Instead of ground state averages, we need the thermal averages

$$\langle X_{\mathbf{q}} X_{-\mathbf{q}} \rangle = \langle P_{\mathbf{q}} P_{-\mathbf{q}} \rangle = \frac{1}{2} (1 + 2b(\omega_{\mathbf{q}})) = \frac{1}{2} \coth \frac{\omega_{\mathbf{q}}}{2T},$$

where $b(\omega_{\mathbf{q}})$ is the Bose distribution function

$$b(x) = \frac{1}{e^{\beta x} + 1}.$$

(**Exercise:** Derive the above result). Therefore, at finite temperature, the order parameter is

$$M(T) = S + \frac{1}{2} - \frac{1}{2N} \sum_{\mathbf{q}} \sqrt{\frac{d + \gamma_{\mathbf{q}}}{d - \gamma_{\mathbf{q}}}} \coth \frac{\omega_{\mathbf{q}}}{2T}. \quad (2.97)$$

We notice that in two-dimensions the contribution of thermal fluctuations is diverging since, for $\omega_{\mathbf{q}} \ll T$,

$$\coth \frac{\omega_{\mathbf{q}}}{2T} \sim \frac{2T}{\omega_{\mathbf{q}}},$$

and the sum behaves like

$$\frac{T}{v} \int \frac{d\mathbf{q}}{|\mathbf{q}|^2},$$

which is singular in two-dimensions. This implies that for $d = 2$ only at T strictly zero there is a true Néel order. For dimensions $d > 2$, Eq. (2.97) allows to estimate the value of the critical temperature T_c above which the order parameter vanishes through the equation $M(T_c) = 0$. Since J is the only dimensional coupling, one easily realize that the Néel critical temperature $T_c \sim J$.

2.7.1 More rigorous derivation: the Holstein-Primakoff transformation

Let us conclude by showing more rigorously how one can derive the spin wave theory. One can readily demonstrate that the following way of writing spin operators in terms of bosonic one (**Holstein-Primakoff transformation**) preserves proper spin commutation relations:

$$S_{\mathbf{R}}^z = (-1)^R [S - d_{\mathbf{R}}^\dagger d_{\mathbf{R}}], \quad (2.98)$$

$$S_{\mathbf{R}}^+ = \frac{1}{2} [1 - (-1)^R] d_{\mathbf{R}}^\dagger \sqrt{2S - \hat{n}_{\mathbf{R}}} + \frac{1}{2} [1 + (-1)^R] \sqrt{2S - \hat{n}_{\mathbf{R}}} d_{\mathbf{R}}, \quad (2.99)$$

$$S_{\mathbf{R}}^- = \frac{1}{2} [1 + (-1)^R] d_{\mathbf{R}}^\dagger \sqrt{2S - \hat{n}_{\mathbf{R}}} + \frac{1}{2} [1 - (-1)^R] \sqrt{2S - \hat{n}_{\mathbf{R}}} d_{\mathbf{R}}, \quad (2.100)$$

where $\hat{n}_{\mathbf{R}} = d_{\mathbf{R}}^\dagger d_{\mathbf{R}}$. Notice that the bosonic vacuum has the properties

$$\langle 0 | S_{\mathbf{R}}^z | 0 \rangle = (-1)^R S, \quad \langle 0 | S_{\mathbf{R}}^+ | 0 \rangle = \langle 0 | S_{\mathbf{R}}^- | 0 \rangle = 0,$$

namely it corresponds to the classical Ne  l state. The square root operators in (2.99) and (2.100) assure that it is not possible to create more than $2S$ bosons at any given site, so that $\langle S_{\mathbf{R}}^z \rangle = -S, \dots, S$ as it should. If one inserts the above expressions in the Heisenberg Hamiltonian and expands it up to order S , the effective Hamiltonian (2.87) is recovered, after moving from bosonic operators to conjugate variables.

Exercises:

- Determine how the specific heat behaves at low energy for the antiferromagnetic Heisenberg Hamiltonian (2.82) in an hypercubic lattice in $d \geq 3$ dimensions.
- Add to the antiferromagnetic Heisenberg Hamiltonian (2.82) with symmetry breaking along the z -direction a magnetic field along the x -direction with Fourier components $B_{\mathbf{q}}$, i.e. a term

$$\delta \hat{H} = - \sum_{\mathbf{q}} B_{-\mathbf{q}} S_{\mathbf{q}}^x \simeq -\sqrt{SN} \sum_{\mathbf{q}} B_{-\mathbf{q}} x_{\mathbf{q}}.$$

Diagonalize the Hamiltonian in the presence of this term and calculate the ground state energy.

- Calculate the spin wave spectrum of the Heisenberg ferromagnetic Hamiltonian

$$\mathcal{H} = -J \sum_{\langle \mathbf{R} \mathbf{R}' \rangle} \mathbf{S}_{\mathbf{R}} \cdot \mathbf{S}_{\mathbf{R}'},$$

with $J > 0$ and where $\langle \mathbf{R} \mathbf{R}' \rangle$ means sum over nearest neighbor sites on an hypercubic lattice in d dimensions.

Chapter 3

Linear Response Theory

In order to access the physical properties of a system, one has to act on it with some external probe. This amounts to add to the unperturbed Hamiltonian \hat{H}_0 a time-dependent perturbation of the general form

$$\hat{V}(t) = \int d\mathbf{x} \hat{A}(\mathbf{x}) v(\mathbf{x}, t), \quad (3.1)$$

where $v(\mathbf{x}, t)$ represents the external probe which couples to the hermitean operator $\hat{A}(\mathbf{x})$. Our scope is to study the effects of $\hat{V}(t)$ on some measurable quantity described e.g. by an operator $\hat{B}(\mathbf{x})$, namely to calculate

$$B(\mathbf{x}, t) \equiv \text{Tr} [\hat{\rho}(t) \hat{B}(\mathbf{x})],$$

being $\hat{\rho}(t)$ the time-dependent density matrix in the presence of the perturbation.

3.1 Linear Response Functions

We assume that the perturbation is switched on at time $t \rightarrow -\infty$. Initially the system is in thermal equilibrium, so that the density matrix

$$\lim_{t \rightarrow -\infty} \hat{\rho}(t) = \hat{\rho}_0, \quad (3.2)$$

with

$$\hat{\rho}_0 = \frac{1}{Z_0} e^{-\beta \hat{H}_0} = \frac{1}{Z_0} \sum_n e^{-\beta E_n} |\phi_n\rangle \langle \phi_n|. \quad (3.3)$$

Here $\hat{H}_0 |\phi_n\rangle = E_n |\phi_n\rangle$ and $Z_0 = \sum_n \exp(-\beta E_n)$. Therefore the time evolution of the density matrix in the presence of $\hat{V}(t)$ is given by

$$\hat{\rho}(t) = \frac{1}{Z_0} \sum_n e^{-\beta E_n} |\phi_n(t)\rangle \langle \phi_n(t)|, \quad (3.4)$$

where

$$i\hbar \frac{\partial}{\partial t} |\phi_n(t)\rangle = [\hat{H}_0 + \hat{V}(t)] |\phi_n(t)\rangle, \quad (3.5)$$

is the Shrödinger equation which determines the evolution of the eigenstates of the unperturbed Hamiltonian in the presence of the perturbation. The meaning of (3.4) is that initially the system is described by a statistical ensemble of sub-systems, each in a given eigenstate of \hat{H}_0 and weighted by the Boltzmann factor. After we switch on the perturbation, $|\phi_n\rangle$ ceases to be an eigenstate of the perturbed Hamiltonian, so it acquires a non-trivial time evolution.

Through Eq. (3.5) one readily finds the equation of motion for the density matrix

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}(t) = [\hat{H}_0 + \hat{V}(t), \hat{\rho}(t)]. \quad (3.6)$$

We introduce the Dirac, also called interaction, representation of the density matrix as

$$\hat{\rho}_D(t) = e^{i\hat{H}_0 t/\hbar} \hat{\rho}(t) e^{-i\hat{H}_0 t/\hbar},$$

which satisfies

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \hat{\rho}_D(t) &= -[\hat{H}_0, \hat{\rho}_D(t)] + e^{i\hat{H}_0 t/\hbar} [\hat{H}_0 + \hat{V}(t), \hat{\rho}(t)] e^{-i\hat{H}_0 t/\hbar} \\ &= [\hat{V}_D(t), \hat{\rho}_D(t)], \end{aligned} \quad (3.7)$$

where

$$\hat{V}_D(t) = \int d\mathbf{x} e^{i\hat{H}_0 t/\hbar} \hat{A}(\mathbf{x}) e^{-i\hat{H}_0 t/\hbar} v(\mathbf{x}, t) = \int d\mathbf{x} \hat{A}(\mathbf{x}, t) v(\mathbf{x}, t),$$

being $\hat{A}(\mathbf{x}, t)$ the Heisenberg evolution of $\hat{A}(\mathbf{x})$ with the unperturbed Hamiltonian. We solve (3.7) perturbatively in v , i.e. $\rho_D(t) = \rho_D^{(0)}(t) + \rho_D^{(1)}(t) + \dots$, where $\rho_D^{(n)}(t)$ contains n -powers of the perturbation. Obviously

$$\lim_{t \rightarrow -\infty} \hat{\rho}_D(t) = \hat{\rho}_0 = \hat{\rho}_D^{(0)}.$$

We will limit our analysis to the linear response, hence we just need the first order term which satisfies

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}_D^{(1)}(t) = [\hat{V}_D(t), \hat{\rho}_D^{(0)}(t)],$$

with solution

$$\hat{\rho}_D^{(1)}(t) = -\frac{i}{\hbar} \int_{-\infty}^t dt' [\hat{V}_D(t'), \hat{\rho}_0]. \quad (3.8)$$

Therefore, at linear order,

$$B(\mathbf{x}, t) = \text{Tr} [\hat{\rho}(t) \hat{B}(\mathbf{x})] = \text{Tr} [\hat{\rho}_D(t) e^{i\hat{H}_0 t/\hbar} \hat{B}(\mathbf{x}) e^{i\hat{H}_0 t/\hbar}]$$

$$\begin{aligned}
&= \text{Tr} \left[\hat{\rho}_D(t) \hat{B}(\mathbf{x}, t) \right] = \text{Tr} \left[\hat{\rho}_0 \hat{B}(\mathbf{x}, t) \right] \\
&\quad + \text{Tr} \left[\hat{\rho}_D^{(1)}(t) \hat{B}(\mathbf{x}, t) \right] \\
&= B(\mathbf{x})_0 + \text{Tr} \left[\hat{\rho}_D^{(1)}(t) \hat{B}(\mathbf{x}, t) \right]
\end{aligned}$$

where we used the fact that

$$\text{Tr} \left[\hat{\rho}_0 \hat{B}(\mathbf{x}, t) \right] = \text{Tr} \left[\hat{\rho}_0 \hat{B}(\mathbf{x}) \right] = B(\mathbf{x})_0,$$

is the unperturbed average value. We then find that the variation of the average value is given by

$$\begin{aligned}
B(\mathbf{x}, t) - B(\mathbf{x})_0 &= -\frac{i}{\hbar} \int_{-\infty}^t dt' \text{Tr} \left\{ \left[\hat{V}_D(t'), \hat{\rho}_0 \right] \hat{B}(\mathbf{x}, t) \right\} \\
&= -\frac{i}{\hbar} \int_{-\infty}^t dt' \int d\mathbf{y} \text{Tr} \left\{ \hat{\rho}_0 \left[\hat{B}(\mathbf{x}, t), \hat{A}(\mathbf{y}, t') \right] \right\} v(\mathbf{y}, t') \\
&= -\frac{i}{\hbar} \int_{-\infty}^{\infty} dt' \int d\mathbf{y} \theta(t - t') \text{Tr} \left\{ \hat{\rho}_0 \left[\hat{B}(\mathbf{x}, t), \hat{A}(\mathbf{y}, t') \right] \right\} v(\mathbf{y}, t') \\
&\equiv \int_{-\infty}^{\infty} dt' \int d\mathbf{y} \chi_{BA}(\mathbf{x}, \mathbf{y}; t - t') v(\mathbf{y}, t'), \tag{3.9}
\end{aligned}$$

with the linear response function defined through

$$\chi_{BA}(\mathbf{x}, \mathbf{y}; t - t') = -\frac{i}{\hbar} \theta(t - t') \langle \left[\hat{B}(\mathbf{x}, t), \hat{A}(\mathbf{y}, t') \right] \rangle, \tag{3.10}$$

where $\langle \dots \rangle$ means a thermal and quantum average with the unperturbed density matrix and we recall that the operators evolve in time with \hat{H}_0 .

Eq. (3.9) shows that, at linear order, the variation of any measurable quantity is obtained through the linear response function (3.10) which is only related to averages on the unperturbed system.

We conclude by noticing that any average of pairs of time-evolved operators in the Heisenberg representation only depends on the time-difference, since the Schrödinger equation is time-translationally invariant. In fact

$$\begin{aligned}
\langle \hat{B}(t) \hat{A}(t') \rangle &= \frac{1}{Z} \text{Tr} \left(e^{-\beta H} e^{i H t / \hbar} \hat{B} e^{-i H t / \hbar} e^{i H t' / \hbar} \hat{A} e^{-i H t' / \hbar} \right) \\
&= \frac{1}{Z} \text{Tr} \left(e^{-\beta H} e^{i H (t-t') / \hbar} \hat{B} e^{-i H (t-t') / \hbar} \hat{A} \right) = \langle \hat{B}(t - t') \hat{A}(0) \rangle \\
&= \frac{1}{Z} \text{Tr} \left(e^{-\beta H} \hat{B} e^{i H (t'-t) / \hbar} \hat{A} e^{-i H (t'-t) / \hbar} \right) = \langle \hat{B}(0) \hat{A}(t' - t) \rangle.
\end{aligned}$$

3.2 Kramers-Kronig relations

Let us now study the analytical properties of the response function in the frequency domain. In the following we drop the space-coordinate dependence of the response function, which is not relevant for what we are going to demonstrate. The response of an operator \hat{A} in the presence of an external probe which couples to \hat{B} is therefore

$$\chi_{AB}(t) = -\frac{i}{\hbar}\theta(t)\langle [\hat{A}(t), \hat{B}] \rangle, \quad (3.11)$$

where

$$\hat{A}(t) = e^{i\frac{\hat{H}_0 t}{\hbar}} \hat{A} e^{-i\frac{\hat{H}_0 t}{\hbar}}.$$

The response function (3.11) vanishes for $t < 0$, which is a consequence of *causality*. We introduce the Fourier transform through

$$\chi_{AB}(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \chi_{AB}(\omega), \quad (3.12)$$

as well as its analytical continuation in the complex frequency plane $\chi_{AB}(z)$. If we assume, as it is always the case, that $\chi_{AB}(z)$ does not diverge exponentially for $|z| \rightarrow \infty$, we can regard (3.12) as the result of a contour integral

$$\chi_{AB}(t) = \oint \frac{dz}{2\pi} e^{-izt} \chi_{AB}(z),$$

where the contour is in the upper half plane for $t < 0$ and in the lower for $t > 0$. The integral catches all poles lying inside the contour. Since $\chi_{AB}(t) = 0$ for $t < 0$, it follows that

- as consequence of causality $\chi_{AB}(z)$ is analytic in the upper half plane. •

Let us now consider the contour drawn in Fig. 3.1. Since there are no poles enclosed by the contour, it is trivially zero the integral

$$\oint_C dz \frac{\chi_{AB}(z)}{\omega - z} = 0. \quad (3.13)$$

On the other hand the above integral is also equal to the line integral along the lower edge, hence

$$\begin{aligned} 0 &= \left\{ \int_{-\infty}^{\omega-\epsilon} + \int_{\omega+\epsilon}^{\infty} \right\} d\omega' \frac{\chi_{AB}(\omega')}{\omega - \omega'} + \oint_{z=\omega+\epsilon \exp(i\theta); \theta \in [\pi, 0]} dz \frac{\chi_{AB}(z)}{\omega - z} \\ &= \mathcal{P} \int_{-\infty}^{\infty} d\omega' \frac{\chi_{AB}(\omega')}{\omega - \omega'} - i \int_{\pi}^0 d\theta \chi_{AB}(\omega + \epsilon e^{i\theta}), \end{aligned}$$

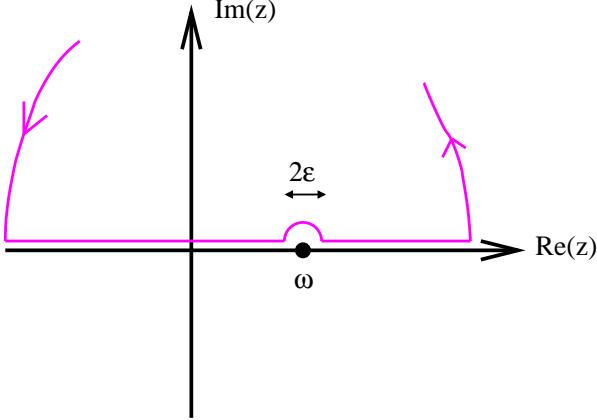


Figure 3.1: Integration contour in Eq. (3.13).

the symbol \mathcal{P} denoting the principal value of the integral. In the limit $\epsilon \rightarrow 0$, the above expression simplifies into

$$\mathcal{P} \int_{-\infty}^{\infty} d\omega' \frac{\chi_{AB}(\omega')}{\omega - \omega'} + i\pi \chi_{AB}(\omega) = 0, \quad (3.14)$$

which implies that

$$\text{Im } \chi_{AB}(\omega) = \mathcal{P} \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\text{Re } \chi_{AB}(\omega')}{\omega - \omega'}, \quad (3.15)$$

$$\text{Re } \chi_{AB}(\omega) = -\mathcal{P} \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\text{Im } \chi_{AB}(\omega')}{\omega - \omega'}, \quad (3.16)$$

known as the Kramers-Kronig relations. Therefore, because of causality, the real and imaginary parts of the response function are not independent. It is possible to rewrite both expressions as

$$\chi_{AB}(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\text{Im } \chi_{AB}(\omega')}{\omega' - \omega - i\eta}, \quad (3.17)$$

with η an infinitesimal positive number.

3.2.1 Symmetries

Let us introduce back the space dependence, so that

$$\chi_{AB}(\mathbf{x}, \mathbf{y}; t - t') = -\frac{i}{\hbar} \theta(t - t') \langle [\hat{A}(\mathbf{x}, t), \hat{B}(\mathbf{y}, t')] \rangle. \quad (3.18)$$

Since both operators are hermitean, it follows that

$$\chi_{AB}(\mathbf{x}, \mathbf{y}; t - t')^* = \frac{i}{\hbar} \theta(t - t') \langle [\hat{B}(\mathbf{y}, t'), \hat{A}(\mathbf{x}, t)] \rangle = \chi_{AB}(\mathbf{x}, \mathbf{y}; t - t'). \quad (3.19)$$

By definition

$$\chi_{AB}(\mathbf{x}, \mathbf{y}; \omega) = \int dt e^{i\omega t} \chi_{AB}(\mathbf{x}, \mathbf{y}; t),$$

therefore, through (3.19), we find that

$$\chi_{AB}(\mathbf{x}, \mathbf{y}; \omega)^* = \int dt e^{-i\omega t} \chi_{AB}(\mathbf{x}, \mathbf{y}; t)^* = \chi_{AB}(\mathbf{x}, \mathbf{y}; -\omega).$$

This implies that

$$\mathcal{R}e \chi_{AB}(\mathbf{x}, \mathbf{y}; \omega) = \frac{1}{2} [\chi_{AB}(\mathbf{x}, \mathbf{y}; \omega) + \chi_{AB}(\mathbf{x}, \mathbf{y}; -\omega)],$$

is even in frequency, while

$$\mathcal{I}m \chi_{AB}(\mathbf{x}, \mathbf{y}; \omega) = \frac{1}{2i} [\chi_{AB}(\mathbf{x}, \mathbf{y}; \omega) - \chi_{AB}(\mathbf{x}, \mathbf{y}; -\omega)],$$

is odd.

3.3 Fluctuation-Dissipation Theorem

Let us introduce other types of correlation functions. The first are the so-called structure factors defined through

$$S_{AB}(\mathbf{x}, \mathbf{y}; t) = \frac{1}{\hbar} \langle \hat{A}(\mathbf{x}, t) \hat{B}(\mathbf{y}) \rangle. \quad (3.20)$$

In addition we introduce the dissipation response function

$$\chi''_{AB}(\mathbf{x}, \mathbf{y}; t) = \frac{1}{2\hbar} \langle [\hat{A}(\mathbf{x}, t), \hat{B}(\mathbf{y})] \rangle = \frac{1}{2} [S_{AB}(\mathbf{x}, \mathbf{y}; t) - S_{BA}(\mathbf{y}, \mathbf{x}; -t)], \quad (3.21)$$

whose meaning will be explained in the following section, as well as the fluctuation one

$$F_{AB}(\mathbf{x}, \mathbf{y}; t) = \frac{1}{2} \langle \{\hat{A}(\mathbf{x}, t), \hat{B}(\mathbf{y})\} \rangle = \frac{\hbar}{2} [S_{AB}(\mathbf{x}, \mathbf{y}; t) + S_{BA}(\mathbf{y}, \mathbf{x}; -t)]. \quad (3.22)$$

One readily verifies that the former is related to the response function through

$$\chi''_{AB}(\mathbf{x}, \mathbf{y}; t) = \frac{i}{2} [\chi_{AB}(\mathbf{x}, \mathbf{y}; t) - \chi_{BA}(\mathbf{y}, \mathbf{x}; -t)],$$

which in the frequency domain reads

$$\chi''_{AB}(\mathbf{x}, \mathbf{y}; \omega) = \frac{i}{2} [\chi_{AB}(\mathbf{x}, \mathbf{y}; \omega) - \chi_{BA}(\mathbf{y}, \mathbf{x}; -\omega)]. \quad (3.23)$$

In particular

$$\chi''_{AA}(\mathbf{x}, \mathbf{x}; \omega) = -\mathcal{Im} \chi_{AA}(\mathbf{x}, \mathbf{x}; \omega). \quad (3.24)$$

Through the definition (3.20) we find that

$$\begin{aligned} S_{BA}(\mathbf{y}, \mathbf{x}; -t) &= \frac{1}{Z_0} \text{Tr} \left(e^{-\beta \hat{H}_0} e^{-i \hat{H}_0 \frac{t}{\hbar}} \hat{B}(\mathbf{y}) e^{i \hat{H}_0 \frac{t}{\hbar}} \hat{A}(\mathbf{x}) \right) \\ &= \frac{1}{Z_0} \text{Tr} \left(e^{-\beta \hat{H}_0} e^{i \hat{H}_0 \frac{(t-i\beta\hbar)}{\hbar}} \hat{A}(\mathbf{x}) e^{-i \hat{H}_0 \frac{(t-i\beta\hbar)}{\hbar}} \hat{B}(\mathbf{y}) \right) \\ &= S_{AB}(\mathbf{x}, \mathbf{y}; t - i\hbar\beta). \end{aligned}$$

Therefore

$$\begin{aligned} S_{BA}(\mathbf{y}, \mathbf{x}; -\omega) &= \int dt e^{-i\omega t} S_{BA}(\mathbf{y}, \mathbf{x}; t) = \int dt e^{i\omega t} S_{BA}(\mathbf{y}, \mathbf{x}; -t) \\ &= \int dt e^{i\omega t} S_{AB}(\mathbf{x}, \mathbf{y}; t - i\hbar\beta) = e^{-\beta\hbar\omega} S_{AB}(\mathbf{x}, \mathbf{y}; \omega), \end{aligned} \quad (3.25)$$

namely

$$\chi''_{AB}(\mathbf{x}, \mathbf{y}; \omega) = \frac{1}{2} S_{AB}(\mathbf{x}, \mathbf{y}; \omega) \left(1 - e^{-\beta\hbar\omega} \right), \quad (3.26)$$

$$F_{AB}(\mathbf{x}, \mathbf{y}; \omega) = \frac{\hbar}{2} S_{AB}(\mathbf{x}, \mathbf{y}; \omega) \left(1 + e^{-\beta\hbar\omega} \right). \quad (3.27)$$

In other words the following relation holds

$$F_{AB}(\mathbf{x}, \mathbf{y}; \omega) = \hbar \coth \left(\frac{\beta\hbar\omega}{2} \right) \chi''_{AB}(\mathbf{x}, \mathbf{y}; \omega), \quad (3.28)$$

which is the so-called fluctuation-dissipation theorem. Indeed, if $\hat{A} = \hat{B}$ and $\mathbf{x} = \mathbf{y}$, $F_{AA}(\mathbf{x}, \mathbf{x}; t = 0)$ is an estimate of the fluctuations of \hat{A} . On the other hand

$$F_{AA}(\mathbf{x}, \mathbf{x}; t = 0) = \int \frac{d\omega}{2\pi} F_{AA}(\mathbf{x}, \mathbf{x}; \omega) \quad (3.29)$$

$$= \hbar \int \frac{d\omega}{2\pi} \coth \left(\frac{\beta\hbar\omega}{2} \right) \chi''_{AA}(\mathbf{x}, \mathbf{x}; \omega), \quad (3.30)$$

which relates the fluctuations to the dissipation.

3.4 Spectral Representation

The spectral representation of the response functions gives instructive information about their physical meaning. Let us start from the structure factor (3.20) which can be written as (in the following we do not explicitly indicate the space dependence)

$$\begin{aligned} S_{AB}(t) &= \frac{1}{\hbar Z} \sum_n e^{-\beta E_n} \langle n | e^{i \hat{H} t / \hbar} \hat{A} e^{-i \hat{H} t / \hbar} \hat{B} | n \rangle \\ &= \frac{1}{\hbar Z} \sum_{nm} e^{-\beta E_n} e^{i(E_n - E_m)t/\hbar} \langle n | \hat{A} | m \rangle \langle m | \hat{B} | n \rangle. \end{aligned}$$

After Fourier transformation we get

$$S_{AB}(\omega) = \frac{2\pi}{Z} \sum_{nm} e^{-\beta E_n} \langle n | \hat{A} | m \rangle \langle m | \hat{B} | n \rangle \delta(\hbar\omega + E_n - E_m). \quad (3.31)$$

The meaning is now self-evident. The matrix element $\langle m | \hat{B} | n \rangle$ is the transition amplitude for the excitation of the initial state $|n\rangle$ into the final one $|m\rangle$ induced by the operator \hat{B} , while $\langle n | \hat{A} | m \rangle$ describes the reverse process but now induced by \hat{A} . The excitation followed by relaxation process is weighted by the Boltzmann factor for the initial state and contributes to $S_{AB}(\omega)$ only if the energy difference $E_m - E_n$ is $\hbar\omega$. Thus $S_{AB}(\omega)$ is a spectral function which measures the transition amplitude for excitations induced by \hat{B} and de-excitation induced by \hat{A} with a given energy $\hbar\omega$.

Through (3.25) we also find that

$$\begin{aligned} \chi''_{AB}(\omega) &= \frac{\pi}{Z} \sum_{nm} e^{-\beta E_n} \left(1 - e^{-\beta \hbar\omega}\right) \langle n | \hat{A} | m \rangle \langle m | \hat{B} | n \rangle \delta(\hbar\omega + E_n - E_m) \\ &= \frac{\pi}{Z} \sum_{nm} \left(e^{-\beta E_n} - e^{-\beta E_m}\right) \langle n | \hat{A} | m \rangle \langle m | \hat{B} | n \rangle \delta(\hbar\omega + E_n - E_m), \end{aligned} \quad (3.32)$$

which means that $\chi''_{AB}(\omega)$ is the transition amplitude for $|n\rangle \rightarrow |m\rangle$ induced by \hat{B} and $|m\rangle \rightarrow |n\rangle$ induced by \hat{A} weighted by the occupation probability

$$p_n = \frac{e^{-\beta E_n}}{Z},$$

of the initial state $|n\rangle$ minus that one

$$p_m = \frac{e^{-\beta E_m}}{Z},$$

of the final state $|m\rangle$. We notice that

$$p_n - p_m = p_n(1 - p_m) - p_m(1 - p_n),$$

namely it is the probability of n being occupied and m empty, minus the opposite. In other words, $\chi''_{AB}(\omega)$ measures the absorption minus the emission probability of an energy $\hbar\omega$, namely the total absorption probability.

Finally, one can analogously derive the spectral representation of the response function χ_{AB} ,

$$\begin{aligned}\chi_{AB}(t) &= -\frac{i}{\hbar}\theta(t)\frac{1}{Z}\sum_{nm}e^{-\beta E_n} \\ &\quad \left[e^{i(E_n-E_m)t/\hbar}\langle n|\hat{A}|m\rangle\langle m|\hat{B}|n\rangle - e^{-i(E_n-E_m)t/\hbar}\langle n|\hat{B}|m\rangle\langle m|\hat{A}|n\rangle\right] \\ &= -\frac{i}{\hbar}\theta(t)\frac{1}{Z}\sum_{nm}\langle n|\hat{A}|m\rangle\langle m|\hat{B}|n\rangle e^{i(E_n-E_m)t/\hbar} \left(e^{-\beta E_n} - e^{-\beta E_m}\right).\end{aligned}$$

For the Fourier transform one has to evaluate the integral

$$-i\int_0^\infty dt e^{i\omega t} e^{i(E_n-E_m)t/\hbar}.$$

Since the perturbation has been assumed to be switched on at very early times, a meaningful regularization of the above integral is

$$-i\int_0^\infty dt e^{i\omega t} e^{i(E_n-E_m)t/\hbar} e^{-\eta t/\hbar} = \frac{\hbar}{\hbar\omega - (E_m - E_n) + i\eta},$$

where η/\hbar is the switching rate of the perturbation, and is taken to be an infinitesimal positive number. As a result we find that

$$\chi_{AB}(\omega) = \frac{1}{Z}\sum_{nm}\langle n|\hat{A}|m\rangle\langle m|\hat{B}|n\rangle \frac{e^{-\beta E_n} - e^{-\beta E_m}}{\hbar\omega - (E_m - E_n) + i\eta}. \quad (3.33)$$

3.5 Power dissipation

Till now we have formally introduced several response functions. In this section and in the following ones we are going to show how those functions emerge in real experiments.

Let us first analyse the power dissipated in the presence of the perturbation. Given our starting assumption about the time-evolution of the density matrix (3.4), it is clear that the entropy defined through the phase space occupied by the statistical ensemble remains constant and equal to the thermal equilibrium one, S_0 . Therefore the system free energy is

$$F(t) = U(t) - TS_0 = (U(t) - U_0) + F_0,$$

so that

$$\frac{\partial F(t)}{\partial t} = \frac{\partial U(t)}{\partial t}.$$

On the other hand, since

$$U(t) = \text{Tr} \left(\hat{\rho}(t) \hat{H}_0 \right),$$

it follows that

$$\begin{aligned} \frac{\partial U(t)}{\partial t} &= -\frac{i}{\hbar} \text{Tr} \left([\hat{H}_0 + \hat{V}(t), \hat{\rho}(t)] \hat{H}_0 \right) \\ &= -\frac{i}{\hbar} \text{Tr} \left(\hat{\rho}(t) [\hat{H}_0, \hat{H}_0 + \hat{V}(t)] \right) \\ &= -\frac{i}{\hbar} \text{Tr} \left(\hat{\rho}(t) [\hat{H}_0, \hat{V}(t)] \right). \end{aligned} \quad (3.34)$$

We assume that the perturbation has the general form

$$\hat{V}(t) = \sum_J \hat{A}_J v_J(t),$$

so that

$$\frac{\partial U(t)}{\partial t} = -\frac{i}{\hbar} \sum_J v_J(t) \text{Tr} \left(\hat{\rho}(t) [\hat{H}_0, \hat{A}_J] \right) = \frac{i}{\hbar} \sum_J v_J(t) \langle [\hat{A}_J, \hat{H}_0] \rangle(t), \quad (3.35)$$

where the last term denotes the average value of the operator within the bracket in the presence of the time-dependent perturbation. We further notice that

$$A_J(t) = \text{Tr} \left(\hat{\rho}(t) \hat{A}_J \right) = \sum_{J'} \int dt' \chi_{JJ'}(t-t') v_{J'}(t'),$$

where

$$\chi_{JJ'}(t-t') = -\frac{i}{\hbar} \theta(t-t') \langle [\hat{A}_J(t), \hat{A}_{J'}(t')] \rangle.$$

Therefore, by recalling that the operators evolve with the unperturbed Hamiltonian, we find that

$$\begin{aligned} i\hbar \sum_{J'} \int dt' \frac{\partial}{\partial t} \chi_{JJ'}(t-t') v_{J'}(t') &= \sum_{J'} \int dt' \delta(t-t') \langle [\hat{A}_J(t), \hat{A}_{J'}(t)] \rangle v_{J'}(t') \\ &\quad - \sum_{J'} \int dt' \frac{i}{\hbar} \theta(t-t') \langle [\hat{A}_J(t), \hat{H}_0], \hat{A}_{J'}(t') \rangle v_{J'}(t') \\ &= \sum_{J'} \langle [\hat{A}_J(t), \hat{A}_{J'}(t)] \rangle v_{J'}(t) + \langle [\hat{A}_J(t), \hat{H}_0] \rangle. \end{aligned}$$

After inserting into (3.35) we finally get

$$\frac{\partial U(t)}{\partial t} = - \sum_{J,J'} \int dt' \frac{\partial}{\partial t} \chi_{JJ'}(t-t') v_J(t) v_{J'}(t')$$

$$-\frac{i}{\hbar} \sum_{J,J'} \langle [\hat{A}_J(t), \hat{A}_{J'}(t)] \rangle v_J(t) v_{J'}(t).$$

The last term vanishes since the commutator is odd by interchanging J with J' , while $v_J(t) v_{J'}(t)$ is even. Hence

$$\frac{\partial U(t)}{\partial t} = - \sum_{J,J'} \int dt' \frac{\partial}{\partial t} \chi_{JJ'}(t-t') v_J(t) v_{J'}(t'). \quad (3.36)$$

Let us write

$$v_J(t) = \frac{1}{2} (v_J e^{-i\omega t} + v_J^* e^{i\omega t}), \quad (3.37)$$

and define the power dissipated within a cycle, W , through

$$W = \frac{\omega}{2\pi} \int_0^{2\pi/\omega} dt \frac{\partial U(t)}{\partial t}. \quad (3.38)$$

By performing the integral and by means of (3.36) and (3.37) we obtain for W the expression:

$$W = i \frac{\omega}{4} \sum_{J,J'} v_J^* v_{J'} [\chi_{JJ'}(\omega) - \chi_{J'J}(-\omega)] = \frac{\omega}{2} \sum_{J,J'} v_J^* \chi''_{JJ'}(\omega) v_{J'}, \quad (3.39)$$

where Eq. (3.23) has been used. The power dissipated during a cycle is proportional to what we defined as the dissipation response function, thus explaining its name. Indeed, as we showed in the previous section, $\chi''_{JJ'}(\omega)$ measures the probability of energy absorption during the process, hence its appearance in Eq. (3.39) it is not unexpected. We notice that, since $W > 0$, it derives that $\omega \chi''_{JJ'}(\omega)$ is a positive-definite quadratic form. In particular

$$\omega \chi''_{JJ}(\omega) = -\omega \operatorname{Im} \chi_{JJ}(\omega) > 0,$$

namely the imaginary part of $\chi_{JJ}(\omega)$ is positive for $\omega < 0$ and negative otherwise.

3.5.1 Absorption/Emission Processes

The power dissipation is related to the absorption minus emission probability. However, there are other measurements where only absorption or emission is revealed. For instance one can shot on a sample with a beam of particles, either photons, neutrons, electrons etc..., and measure the absorption probability of an energy $\hbar\omega$. If the coupling between the beam and the sample is represented by an operator \hat{A} , the Fermi golden rule tells us that the absorption rate per unit time of an ensamble at thermal equilibrium is

$$P_A(\omega) = \frac{2\pi}{Z} \sum_{if} e^{-\beta E_i} \left| \langle f | \hat{A} | i \rangle \right|^2 \delta(\hbar\omega + E_i - E_f) = S_{AA}(\omega), \quad (3.40)$$

which enlights the meaning of the structure factors.

3.5.2 Thermodynamic Susceptibilities

Let us consider again a perturbation of the form

$$\hat{V}(t) = \sum_J \int d\mathbf{x} \hat{A}_J(\mathbf{x}) v_J(\mathbf{x}, t).$$

Let us further assume that the only time-dependence of the external probes $v_J(\mathbf{x}, t)$ comes from a very slow switching rate (*adiabatic switching*) which just sets the proper regularization of time-integrals as in Eq. (3.33). Hence, for times far away from the time at which the perturbation is switched on, the external probes become constant in time, $v_J(\mathbf{x}, t) = v_J(\mathbf{x})$, and the thermodynamic averages lose any time-dependence. In this limit

$$\begin{aligned} A_J(\mathbf{x}) - A_J(\mathbf{x})_0 &= \sum_{J'} \int_{-\infty}^{\infty} dt' \int d\mathbf{y} \chi_{JJ'}(\mathbf{x}, \mathbf{y}; t - t') v_{J'}(\mathbf{y}) \\ &= \sum_{J'} \int d\mathbf{y} \chi_{JJ'}(\mathbf{x}, \mathbf{y}; \omega = 0) v_{J'}(\mathbf{y}). \end{aligned} \quad (3.41)$$

Let us now consider a generically perturbed Hamiltonian of the form

$$\hat{H} = \hat{H}_0 + \sum_J \int d\mathbf{y} \hat{A}_J(\mathbf{y}) v_J(\mathbf{y}),$$

which therefore admits stationary eigenstates. The perturbed free-energy turns out to be a functional of the external fields $v_J(\mathbf{y})$, $F = F[v_J(\mathbf{y})]$. Standard thermodynamics tells us that

$$\langle \hat{A}_J(\mathbf{x}) \rangle = \frac{\delta F}{\delta v_J(\mathbf{x})},$$

which is in general different from its average value, $\langle \hat{A}_J(\mathbf{x}) \rangle_0$, in the absence of external fields. For very small external fields one finds at linear order that

$$\langle \hat{A}_J(\mathbf{x}) \rangle - \langle \hat{A}_J(\mathbf{x}) \rangle_0 = \sum_{J'} \int d\mathbf{y} \left(\frac{\delta^2 F}{\delta v_J(\mathbf{x}) \delta v_{J'}(\mathbf{y})} \right)_{v=0} v_{J'}(\mathbf{y}), \quad (3.42)$$

where the second derivatives of the unperturbed free-energy are the so-called thermodynamic susceptibilities. Comparing (3.42) with (3.41) one obtains that

$$\left(\frac{\delta^2 F}{\delta v_J(\mathbf{x}) \delta v_{J'}(\mathbf{y})} \right)_{v=0} = \chi_{JJ'}(\mathbf{x}, \mathbf{y}; \omega = 0), \quad (3.43)$$

which relates thermodynamic susceptibilities to the response functions at zero frequency. Notice that thermodynamic stability implies that $-\chi_{JJ'}(\mathbf{x}, \mathbf{y}; \omega = 0)$ is positive definite.

Exercises

- (1) Consider a free electron Hamiltonian

$$\mathcal{H}_0 = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma},$$

in the presence of a Zeeman splitting due to a slowly varying magnetic field oriented along the z -direction $B(\mathbf{q}, t)$. The perturbation is

$$V(\mathbf{q}, t) = \frac{1}{V} \mu_B g B(\mathbf{q}, t) \sigma_{-\mathbf{q}},$$

where V is the volume, μ_B the Bohr magneton, $g \simeq 2$ the electron gyromagnetic ratio and $\sigma_{\mathbf{q}}$ the spin density operator at momentum \mathbf{q} defined through

$$\sigma_{\mathbf{q}} = \frac{1}{2} \sum_{\mathbf{k}} \left(c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}+\mathbf{q}\uparrow} - c_{\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}+\mathbf{q}\downarrow} \right).$$

By linear response theory, the average of the spin-density operator at momentum \mathbf{q} is

$$\langle \sigma_{\mathbf{q}} \rangle(t) = \int dt' \chi(\mathbf{q}, t - t') (g\mu_B B(\mathbf{q}, t')),$$

where

$$\chi(\mathbf{q}, t - t') = -\frac{i}{\hbar} \frac{1}{V} \theta(t - t') \langle [\sigma_{\mathbf{q}}(t), \sigma_{-\mathbf{q}}] \rangle,$$

is the magnetic response function per unit volume. (Prove that for any $\mathbf{p} \neq \mathbf{q}$ $\langle [\sigma_{\mathbf{p}}(t), \sigma_{-\mathbf{q}}] \rangle = 0$, so that only the Fourier component \mathbf{q} is affected by the magnetic field.)

- Find the formal expression of

$$\chi(\mathbf{q}, \omega) = \int dt e^{i\omega t} \chi(\mathbf{q}, t).$$

- Calculate the magnetic susceptibility, namely

$$\chi = \lim_{\mathbf{q} \rightarrow 0} \chi(\mathbf{q}, \omega = 0),$$

at zero temperature in terms of the density of states

$$N(\epsilon) = \frac{1}{V} \sum_{\mathbf{k}} \delta(\epsilon - \epsilon_{\mathbf{k}}).$$

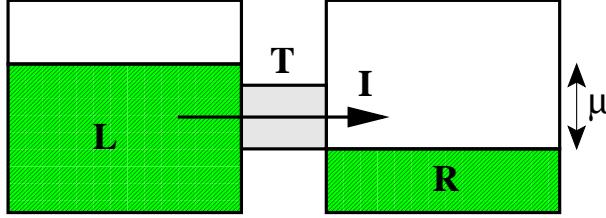


Figure 3.2: Geometry of the tunneling problem (2).

- Prove and discuss that

$$\chi(\mathbf{q} = \mathbf{0}, \omega) = 0.$$

- (2) Consider two disconnected metallic leads, a right one (R) and a left one (L), see Fig. 3.2, described by the unperturbed Hamiltonian

$$\mathcal{H}_0 = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} \left(c_{R\mathbf{k}\sigma}^\dagger c_{R\mathbf{k}\sigma} + c_{L\mathbf{k}\sigma}^\dagger c_{L\mathbf{k}\sigma} \right).$$

At some time, a voltage bias V is applied, implying that the two leads are kept at different chemical potential, i.e. that the following perturbation is added to the Hamiltonian

$$V_\mu = \frac{\mu}{2} \sum_{\mathbf{k}\sigma} \left(c_{R\mathbf{k}\sigma}^\dagger c_{R\mathbf{k}\sigma} - c_{L\mathbf{k}\sigma}^\dagger c_{L\mathbf{k}\sigma} \right) = \frac{\mu}{2} (N_R - N_L),$$

with $\mu = eV$. At the same time a tunnelling between the two leads is switched on, which is described by the additional perturbation

$$V_T = - \sum_{\mathbf{k}\sigma} T(\epsilon_{\mathbf{k}}, \epsilon_{\mathbf{p}}) c_{R\mathbf{k}\sigma}^\dagger c_{L\mathbf{p}\sigma} + H.c.,$$

where we further assume that the tunneling amplitudes $T(\epsilon_{\mathbf{k}}, \epsilon_{\mathbf{p}})$ depends only on the energy. Therefore the fully perturbed Hamiltonian is

$$\mathcal{H} = \mathcal{H}_0 + V_\mu + V_T. \quad (3.44)$$

- Using the Heisenberg equation of motion with the Hamiltonian (3.44), calculate the expression of the operator of the current flowing from the L to the R lead, which is defined through

$$\mathcal{I} = \frac{\partial}{\partial t} (N_R - N_L) = -\frac{i}{\hbar} [(N_R - N_L), \mathcal{H}].$$

- Extending the derivation of the linear response up to second order in the perturbation, calculate the average value of the current $I = \langle \mathcal{I} \rangle$. (One needs the second order density matrix $\hat{\rho}^{(2)}$ in the perturbation $V_\mu + V_T$, and in particular the mixed term which derives from $V_\mu V_T$.) For the explicit calculation it is convenient to introduce the density of states $N(\epsilon)$, which is by definition equal for the L and R leads.

Chapter 4

Hartree-Fock Approximation

In this chapter we describe the simplest approximate technique to study a model of interacting fermions: the Hartree-Fock approximation. This technique is variational and can be applied both at zero and at finite temperature. Essentially within the Hartree-Fock approximation the effects of the particle-particle interaction are simulated by an effective external field acting on the particles which is self-consistently generated by the same particles. This is also the reason why the Hartree-Fock approximation is a Mean Field theory.

The main body is devoted to the Hartree-Fock approximation for interacting fermions. In the last Section the case of bosons is briefly discussed in connection with superfluidity.

4.1 Hartree-Fock Approximation for Fermions at Zero Temperature

The Hartree-Fock (HF) approximation at zero temperature consists in

- searching for a Slater determinant which minimizes the total energy.

Since in general the ground state wavefunction is not a single Slater determinant, the HF approach is variational hence the HF energy is an upper bound to the true ground state energy.

The trial HF wavefunction is a Slater determinant, namely

$$\Phi_{HF}(x_1, \dots, x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(x_1) & \cdots & \phi_1(x_N) \\ \phi_2(x_1) & \cdots & \phi_2(x_N) \\ \vdots & \ddots & \vdots \\ \phi_N(x_1) & \cdots & \phi_N(x_N) \end{vmatrix}, \quad (4.1)$$

where N is the electron number and the single particle wavefunctions $\phi_i(x)$ are for the meanwhile

unknown. They are assumed to belong to a complete set of orthonormal wavefunctions

$$\int dx \phi_i(x)^* \phi_j(x) = \delta_{ij}. \quad (4.2)$$

The Hamiltonian in first quantization is given by

$$\hat{H} = \sum_{i=1}^N T(x_i, p_i) + \frac{1}{2} \sum_{i \neq j} U(x_i, x_j),$$

where

$$T(x, p) = -\frac{\hbar^2}{2m} \nabla^2 + V(x)$$

is a single particle contribution including the kinetic energy as well as a potential term.

The average value of the Hamiltonian over the wavefunction (4.1) is

$$E_{HF} = \frac{\langle \Phi_{HF} | \hat{H} | \Phi_{HF} \rangle}{\langle \Phi_{HF} | \Phi_{HF} \rangle}. \quad (4.3)$$

One has to impose that the variation of E_{HF} vanishes upon varying the trial wavefunction, keeping it still of the form of a Slater determinant. Most generally, this amounts to change one of the single particle wavefunctions, namely

$$\phi_i(x) \rightarrow \mathcal{N}_i (\phi_i(x) + \delta\phi_i(x)). \quad (4.4)$$

Clearly, if the variation $\delta\phi_i(x)$ has a finite overlap with anyone of the $\phi_k(x)$'s already present in (4.1), the Slater determinant does not change, hence such a variation is irrelevant. Therefore the only meaningful possibility is that

$$\delta\phi_i(x) = \eta \phi_j(x), \quad (4.5)$$

where η is an infinitesimal quantity and ϕ_j belongs to the set of wavefunctions (4.2) but does not appear in (4.1), namely $j > N$. The normalization \mathcal{N}_i in Eq. (4.4) is given by

$$\mathcal{N}_i^{-2} = \int dx (\phi_i(x)^* + \eta^* \phi_j(x)^*) (\phi_i(x) + \eta \phi_j(x)) = 1 + |\eta|^2.$$

Therefore $\mathcal{N}_i \simeq 1$ at linear order in η . This implies that also the normalization of the Slater determinant $\Phi_{HF} + \eta \delta\Phi_{HF}$ remains one at linear order in η , hence

$$\begin{aligned} \delta E_{HF} &= \eta^* \langle \delta\Phi_{HF} | \hat{H} | \Phi_{HF} \rangle + \eta \langle \Phi_{HF} | \hat{H} | \delta\Phi_{HF} \rangle \\ &= \mathcal{R}e \eta \mathcal{R}e \langle \delta\Phi_{HF} | \hat{H} | \Phi_{HF} \rangle + \mathcal{I}m \eta \mathcal{I}m \langle \delta\Phi_{HF} | \hat{H} | \Phi_{HF} \rangle = 0. \end{aligned}$$

Since η is an arbitrary infinitesimal number, this implies that

$$\mathcal{R}e\langle\delta\Phi_{HF}|\hat{H}|\Phi_{HF}\rangle = \mathcal{I}m\langle\delta\Phi_{HF}|\hat{H}|\Phi_{HF}\rangle = 0,$$

namely

$$\langle\delta\Phi_{HF}|\hat{H}|\Phi_{HF}\rangle = 0. \quad (4.6)$$

Let us rephrase everything in second quantization. We associate to any of the wavefunctions $\phi_i(x)$ an annihilation and a creation operator, c_i and c_i^\dagger , respectively. The wave-function (4.1) is given by

$$|\Phi_{HF}\rangle = \prod_{i=1}^N c_i^\dagger |0\rangle,$$

while the variation

$$|\delta\Phi_{HF}\rangle = c_j^\dagger c_i |\Phi_{HF}\rangle,$$

with $j > N$ while $i \leq N$. The Hamiltonian in second quantized form is given by

$$\hat{H} = \sum_{ij} t_{ij} c_i^\dagger c_j + \frac{1}{2} \sum_{ijkl} U_{ijkl} c_i^\dagger c_j^\dagger c_k c_l, \quad (4.7)$$

where the parameters are the matrix elements over the basis set (4.2). What we need to solve is therefore the equation

$$\langle\Phi_{HF}|c_i^\dagger c_j \hat{H}|\Phi_{HF}\rangle = 0,$$

where $i \leq N$ and $j > N$. For that we need the following two equalities, which can be easily derived:

$$\begin{aligned} & \sum_{kl} t_{kl} \langle\Phi_{HF}|c_i^\dagger c_j c_k^\dagger c_l|\Phi_{HF}\rangle = t_{ji} \\ & \frac{1}{2} \sum_{klmn} U_{klmn} \langle\Phi_{HF}|c_i^\dagger c_j c_k^\dagger c_l c_m c_n|\Phi_{HF}\rangle \\ &= \frac{1}{2} \sum_{m=1}^N U_{jmim} + U_{mjim} - U_{jmim} - U_{mjmi} \\ &= \sum_{m=1}^N U_{jmim} - U_{jmim}, \end{aligned}$$

where the last expression comes from the symmetry relation

$$U_{ijkl} = U_{jilk}.$$

Eq. (4.6) implies that

$$t_{ji} + \sum_{m=1}^N U_{jmmi} - U_{jmim} = 0, \quad (4.8)$$

if $j > N$ and $i \leq N$. In other words, the Slater determinant which minimizes the total energy is constructed by single particle wavefunctions ϕ_i 's which have matrix elements obeying (4.8). Let us suppose that we have found instead a set of wavefunctions ϕ_i 's satisfying

$$t_{ji} + \sum_{m=1}^N U_{jmmi} - U_{jmim} = \epsilon_i \delta_{ij}. \quad (4.9)$$

This set automatically satisfies also (4.8), hence it does solve our variational problem. In first quantization Eq.(4.9) reads

$$T(x, p) \phi_i(x) + \sum_{m=1}^N \int dy U(x, y) (\phi_m(y)^* \phi_m(y) \phi_i(x) - \phi_m(y)^* \phi_m(x) \phi_i(y)) = \epsilon_i \phi_i(x), \quad (4.10)$$

which is the standard Hartree-Fock set of equations.

Notice that there might be several Slater determinants built up using N of the wavefunctions solving (4.9) which would satisfy the HF variational principle. Among them one has to find the Slater determinant which makes minimum the total energy for N electrons, which can be easily found to be

$$\begin{aligned} E_{HF}(N) &= \langle \Phi_{HF} | \hat{H} | \Phi_{HF} \rangle = \sum_{i=1}^N t_{ii} + \frac{1}{2} \sum_{i,m=1}^N U_{immi} - U_{imim} \\ &= \sum_{i=1}^N \epsilon_i - \frac{1}{2} \sum_{i,m=1}^N U_{immi} - U_{imim}. \end{aligned} \quad (4.11)$$

Notice that, if for $N - 1$ particles the Hartree-Fock single-particle wavefunctions stay approximately invariant, then

$$\begin{aligned} E_{HF}(N-1) &\simeq \sum_{i=1}^{N-1} t_{ii} + \frac{1}{2} \sum_{i,m=1}^{N-1} U_{immi} - U_{imim} \\ &= \sum_{i=1}^N t_{ii} (1 - \delta_{iN}) + \frac{1}{2} \sum_{i,m=1}^N (U_{immi} - U_{imim}) (1 - \delta_{iN}) (1 - \delta_{mN}) \\ &= E_{HF}(N) - \epsilon_N, \end{aligned} \quad (4.12)$$

showing that the Hartree-Fock single particle energies correspond approximately to the ionization energies.

4.1.1 Alternative approach

The Hartree-Fock equations (4.10) are complicated non-linear integral-differential equations. This is especially true if one does not impose any constraint on the form of the variational Slater determinant dictated for instance by the symmetry properties of the Hamiltonian, what is called *unrestricted Hartree-Fock approximation*. However, very often one expects that the true ground state has well defined properties under symmetry transformations which leave the Hamiltonian invariant. For instance, if the Hamiltonian is translationally and spin-rotationally invariant, one may expect that the true ground state is an eigenstate of the total spin and of the total momentum. For this reason one would like to search for a variational wavefunction within the subspace of Slater determinants which are eigenstates of the total spin and momentum. This amounts to impose symmetry constraints on the general form (4.1) of the variational wavefunction. Yet, this is not a simple task if one keeps working within first quantization. The second quantization approach to the Hartree-Fock approximation which we describe in the following has the big advantage to allow an easy implementation of such symmetry constraints.

Let us suppose we have our Hamiltonian written in a basis of single particle wavefunctions $\{\phi_\alpha(x)\}$ which is more convenient to work with (for instance Bloch waves)

$$\hat{H} = \sum_{\alpha\beta} t_{\alpha\beta} c_\alpha^\dagger c_\beta + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} U_{\alpha\beta\gamma\delta} c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta. \quad (4.13)$$

Our scope is to find the basis $\{\phi_i(x)\}$ which solves the Hartree-Fock equations (4.9). The Hartree-Fock wavefunction (4.1), being a Slater determinant, should be the ground state of a single-particle Hamiltonian, which we define as \hat{H}_{HF} . We write such an Hamiltonian in the following general form

$$\begin{aligned} \hat{H}_{HF} &= \sum_{\alpha\beta} t_{\alpha\beta} c_\alpha^\dagger c_\beta + \sum_{\alpha\beta\gamma\delta} c_\alpha^\dagger c_\beta \Delta_{\gamma\delta} (U_{\alpha\gamma\delta\beta} - U_{\alpha\gamma\beta\delta}) \\ &= \sum_{\alpha\beta} c_\alpha^\dagger \left[t_{\alpha\beta} + \sum_{\gamma\delta} \Delta_{\gamma\delta} (U_{\alpha\gamma\delta\beta} - U_{\alpha\gamma\beta\delta}) \right] c_\beta \\ &\equiv \sum_{\alpha\beta} c_\alpha^\dagger (t_{\alpha\beta} + h_{\alpha\beta}) c_\beta, \end{aligned} \quad (4.14)$$

where we have introduced a set of unknown variational parameters satisfying $\Delta_{\alpha\beta} = \Delta_{\beta\alpha}^*$, for the Hamiltonian to be hermitean, or equivalently a set of unknown external fields $h_{\alpha\beta}$. The ignorance about the basis set $\{\phi_i(x)\}$ is reflected in the ignorance about the Δ 's. Since \hat{H}_{HF} is quadratic, it can be diagonalized by a unitary transformation

$$c_\alpha = \sum_i \mathcal{U}_{\alpha i} c_i, \quad c_\alpha^\dagger = \sum_i c_i^\dagger \mathcal{U}_{i\alpha}^\dagger,$$

with $\mathcal{U}\mathcal{U}^\dagger = 1$. The above unitary transformation depends parametrically on the Δ 's, i.e. $\mathcal{U} = \mathcal{U}[\Delta]$. In terms of the eigen-operators

$$\hat{H}_{HF} = \sum_i \epsilon_i c_i^\dagger c_i.$$

The ground state, if $\epsilon_1 \leq \epsilon_2 \leq \dots$, is simply

$$|\Phi_{HF}\rangle = \prod_{i=1}^N c_i^\dagger |0\rangle,$$

and by definition has to coincide with the Hartree-Fock wavefunction (4.1).

Through Eq. (4.9) this leads to the equation

$$\begin{aligned} \delta_{ij}\epsilon_i &= \sum_{\alpha\beta} \mathcal{U}_{i\alpha}^\dagger (t_{\alpha\beta} + h_{\alpha\beta}) \mathcal{U}_{\beta j} \\ &= \sum_{\alpha\beta} \mathcal{U}_{i\alpha}^\dagger \left[t_{\alpha\beta} + \sum_{\gamma\delta} \Delta_{\gamma\delta} (U_{\alpha\gamma\delta\beta} - U_{\alpha\gamma\beta\delta}) \right] \mathcal{U}_{\beta j} \\ &= t_{ij} + \sum_{m=1}^N U_{immj} - U_{imjm}. \end{aligned} \quad (4.15)$$

We notice that the unitary transformation

$$c_\alpha = \sum_i \mathcal{U}_{\alpha i} c_i,$$

implies that the corresponding wavefunctions transform like

$$\begin{aligned} \phi_i(x) &= \sum_\alpha \mathcal{U}_{\alpha i} \phi_\alpha(x), \\ \phi_i(x)^* &= \sum_\alpha \mathcal{U}_{i\alpha}^\dagger \phi_\alpha(x)^*. \end{aligned}$$

Therefore, for instance,

$$\sum_{\alpha\beta} \mathcal{U}_{i\alpha}^\dagger t_{\alpha\beta} \mathcal{U}_{\beta j} = \int dx \left(\sum_\alpha \mathcal{U}_{i\alpha}^\dagger \phi_\alpha(x)^* \right) T(x, p) \left(\sum_\beta \mathcal{U}_{\beta j} \phi_\beta(x) \right) = t_{ij},$$

which shows the equivalence of the first term in (4.15).

By analogy, we write

$$\Delta_{\alpha\beta} = \sum_{ij} \mathcal{U}_{i\alpha}^\dagger \mathcal{U}_{\beta j} \Delta_{ij}, \quad (4.16)$$

so that the second term in (4.15) reads

$$\begin{aligned} & \sum_{\alpha\beta\gamma\delta} \mathcal{U}_{i\alpha}^\dagger [\Delta_{\gamma\delta} (U_{\alpha\gamma\delta\beta} - U_{\alpha\gamma\beta\delta})] \mathcal{U}_{\beta j} \\ &= \sum_{kl} \Delta_{kl} \sum_{\alpha\beta\gamma\delta} \mathcal{U}_{i\alpha}^\dagger \mathcal{U}_{k\gamma}^\dagger (U_{\alpha\gamma\delta\beta} - U_{\alpha\gamma\beta\delta}) \mathcal{U}_{\delta l} \mathcal{U}_{\beta j} \\ &= \sum_{kl} \Delta_{kl} (U_{iklj} - U_{ikjl}). \end{aligned}$$

For Eq. (4.15) to be satisfied, one should impose the following condition

$$\sum_{kl} \Delta_{kl} (U_{iklj} - U_{ikjl}) = \sum_{m=1}^N (U_{immj} - U_{imjm}),$$

which is satisfied if

$$\Delta_{kl} = \delta_{kl} n_k, \quad (4.17)$$

where n_k is the occupation number in the wavefunction (4.1), namely $n_k = 1$ if $k \leq N$ and zero otherwise. This is the condition one has to impose for the Hamiltonian H_{HF} to have as ground state just the desired Hartree-Fock wavefunction (4.1).

In terms of the original variational parameters $\Delta_{\alpha\beta}$ this condition implies, from (4.16), that

$$\Delta_{\alpha\beta} = \sum_{i=1}^N \mathcal{U}_{i\alpha}^\dagger [\Delta] \mathcal{U}_{\beta i} [\Delta]. \quad (4.18)$$

Since the unitary transformation depends parametrically on the $\Delta_{\alpha\beta}$, (4.18) is a self-consistency equation whose solution is perfectly equivalent to the solution of the full Hartree-Fock set of equations (4.9).

We observe that (4.17) is also equivalent to

$$\Delta_{kl} \equiv \langle \Phi_{HF} | c_k^\dagger c_l | \Phi_{HF} \rangle = \delta_{kl} n_k.$$

Upon inserting this equivalence into (4.16) we get

$$\Delta_{\alpha\beta} = \sum_{ij} \mathcal{U}_{i\alpha}^\dagger \mathcal{U}_{\beta j} \langle \Phi_{HF} | c_i^\dagger c_j | \Phi_{HF} \rangle = \langle \Phi_{HF} | c_\alpha^\dagger c_\beta | \Phi_{HF} \rangle. \quad (4.19)$$

This is our final result. It implies that the variational parameters $\Delta_{\alpha\beta}$ which define the Hamiltonian Eq. (4.14) have to be chosen as the average values of the bilinear operators $c_\alpha^\dagger c_\beta$ on the

ground state of the same Hamiltonian H_{HF} , in order for this ground state to be the Hartree-Fock wavefunction (4.1).

The above alternative Hartree-Fock scheme has a big advantage since one can impose physical constraints directly on the variational parameters due to the fact that they also represent quantum average values through

$$\Delta_{\alpha\beta} = \langle \Phi_{HF} | c_{\alpha}^{\dagger} c_{\beta} | \Phi_{HF} \rangle.$$

In this way one can reduce their number and consequently the computational effort.

Let us consider a very simple example. Suppose the Hamiltonian (4.13) is invariant under spin rotational symmetry. The basis-set wavefunctions are labelled by $\alpha = (a, \sigma)$, where σ is the spin. The variational parameters are, accordingly,

$$\Delta_{a\sigma, b\sigma'} = \langle \Phi_{HF} | c_{a\sigma}^{\dagger} c_{b\sigma'} | \Phi_{HF} \rangle.$$

We want to restrict our Hartree-Fock analysis to the subspace spanned by eigenstates of the total z -component of the spin operator. In this case clearly

$$\Delta_{a\uparrow, b\downarrow} = \Delta_{a\downarrow, b\uparrow} = 0.$$

We end by noticing that the Hartree-Fock total-energy is equivalently given by

$$E_{HF} = \sum_{i=1}^N \epsilon_i - \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \Delta_{\alpha\beta} \Delta_{\gamma\delta} (U_{\alpha\gamma\delta\beta} - U_{\alpha\gamma\beta\delta}). \quad (4.20)$$

Clearly, among all possible Slater determinants, E_{HF} is minimized only by the true Hartree-Fock solution. This suggests still another way of deriving the Hartree-Fock equations. Namely the self-consistency condition (4.19) can be straightforwardly derived by the minimal condition

$$\frac{\delta E_{HF}}{\delta \Delta_{\alpha\beta}} = 0. \quad (4.21)$$

Let us conclude this section by summarizing the main result.

Given the interacting Hamiltonian

$$\hat{H} = \sum_{\alpha\beta} t_{\alpha\beta} c_{\alpha}^{\dagger} c_{\beta} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} U_{\alpha\beta\gamma\delta} c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\gamma} c_{\delta},$$

then the Hartree-Fock variational wavefunction $|\Phi_{HF}\rangle$ is the ground state of the single particle Hamiltonian

$$\hat{H}_{HF} = \sum_{\alpha\beta} t_{\alpha\beta} c_{\alpha}^{\dagger} c_{\beta} + \sum_{\alpha\beta\gamma\delta} c_{\alpha}^{\dagger} c_{\beta} \Delta_{\gamma\delta} (U_{\alpha\gamma\delta\beta} - U_{\alpha\gamma\beta\delta})$$

where the parameters $\Delta_{\alpha\beta}$ have to be determined self-consistently by imposing that

$$\Delta_{\alpha\beta} = \langle \Phi_{HF} | c_{\alpha}^{\dagger} c_{\beta} | \Phi_{HF} \rangle.$$

4.2 Hartree-Fock approximation for fermions at finite temperature

A variational approach of the Hartree-Fock type can also be implemented at finite temperature as a variational minimization of the free energy. Before presenting the method, it is necessary to introduce some preliminary results.

4.2.1 Preliminaries

Let us consider a generic Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{V},$$

where \hat{H}_0 is the unperturbed Hamiltonian while \hat{V} is the perturbation, e.g. the interaction, which does not commute with \hat{H}_0 . The partition function is defined through

$$\mathcal{Z} = e^{-\beta F} = \text{Tr} \left(e^{-\beta \hat{H}} \right). \quad (4.22)$$

We assume that the free energy can be expanded in powers of the perturbation, namely

$$F = \sum_{n=0} F^{(n)},$$

where $F^{(n)}$ contains n -powers of \hat{V} .

Let us define for real τ 's

$$e^{-\hat{H}\tau} = e^{-\hat{H}_0\tau} \hat{S}(\tau), \quad (4.23)$$

implying that

$$\hat{S}(\tau) = e^{\hat{H}_0\tau} e^{-\hat{H}\tau}.$$

From this expression it follows that

$$\begin{aligned} \frac{\partial \hat{S}}{\partial \tau} &= e^{\hat{H}_0\tau} (\hat{H}_0 - \hat{H}) e^{-\hat{H}\tau} \\ &= -e^{\hat{H}_0\tau} \hat{V} e^{-\hat{H}_0\tau} e^{\hat{H}_0\tau} e^{-\hat{H}\tau} = -\hat{V}(\tau) \hat{S}(\tau), \end{aligned} \quad (4.24)$$

where we define the unperturbed evolution (Dirac or interaction representation) in imaginary time as

$$\hat{V}(\tau) = e^{\hat{H}_0\tau} \hat{V} e^{-\hat{H}_0\tau}.$$

The equation of motion satisfied by the S -function allows a very simple perturbative expansion. The 0-th order $\hat{S}^{(0)} = 1$ since at this order $\hat{H} = \hat{H}_0$. Moreover, the boundary condition at

$\tau = 0$ is $\hat{S}(0) = 1$, implying that all $\hat{S}^{(n)}(\tau = 0) = 0$ for $n > 0$, since already $S^{(0)} = 1$ and, for any n and τ , $\hat{S}^{(n)}(\tau) > 0$. The first order term satisfies

$$\frac{\partial \hat{S}^{(1)}}{\partial \tau} = -\hat{V}(\tau) \hat{S}^{(0)} = -\hat{V}(\tau).$$

The solution with the appropriate boundary condition is

$$\hat{S}^{(1)}(\tau) = - \int_0^\tau d\tau_1 \hat{V}(\tau_1). \quad (4.25)$$

For a generic n , the equation of motion reads

$$\frac{\partial \hat{S}^{(n)}}{\partial \tau} = -\hat{V}(\tau) \hat{S}^{(n-1)},$$

whose solution can be iteratively found starting from the expression of $\hat{S}^{(1)}$, and reads

$$\hat{S}^{(n)}(\tau) = (-1)^n \int_0^\tau d\tau_n \int_0^{\tau_n} d\tau_{n-1} \dots \int_0^{\tau_2} d\tau_1 \hat{V}(\tau_n) \hat{V}(\tau_{n-1}) \dots \hat{V}(\tau_1). \quad (4.26)$$

We can rewrite this term as $1/n!$ times the sum of all the terms which are obtained by permuting the n -indices. This allows us to formally write

$$\hat{S}^{(n)}(\tau) = \frac{(-1)^n}{n!} \int_0^\tau \prod_{i=1}^n d\tau_i T_\tau \left(\hat{V}(\tau_1) \hat{V}(\tau_2) \dots \hat{V}(\tau_n) \right), \quad (4.27)$$

where we have introduced the so-called time-ordered product of operators, T_τ , which is defined as follows:

- the time-ordered product T_τ of several operators at different (imaginary) times is the product where the operators are ordered in such a way that those at later times appear on the left of those at earlier times. If some of those operators are fermionic-like, namely contain odd number of fermionic operators, the result has to be multiplied by $(-1)^P$, where P is the order of the permutation needed to bring the original sequence of only the fermionic operators into the time-ordered one.

For instance the time-ordered product of two operators $\hat{A}_1(\tau_1)$ and $\hat{A}_2(\tau_2)$ is

$$T_\tau \left(\hat{A}(\tau_1) \hat{A}(\tau_2) \right) = \theta(\tau_1 - \tau_2) \hat{A}(\tau_1) \hat{A}(\tau_2) \pm \theta(\tau_2 - \tau_1) \hat{A}(\tau_2) \hat{A}(\tau_1),$$

where the $-$ sign has to be used if both operators are fermionic-like.

Having introduced the time-ordered product, we can write the general expression for the S -operator as

$$\hat{S}(\tau) = \text{Tr} \left(e^{-\int_0^\tau d\tau' \hat{V}(\tau')} \right). \quad (4.28)$$

Coming back to the partition function, it can be rewritten as

$$\begin{aligned} \mathcal{Z} &= \text{Tr} \left(e^{-\beta \hat{H}} \right) = \text{Tr} \left(e^{-\beta \hat{H}_0} \hat{S}(\beta) \right) \\ &= \mathcal{Z}_0 \frac{1}{\mathcal{Z}_0} \text{Tr} \left(e^{-\beta \hat{H}_0} \hat{S}(\beta) \right) = \mathcal{Z}_0 \langle \hat{S}(\beta) \rangle_0, \end{aligned} \quad (4.29)$$

where

$$\mathcal{Z}_0 = \text{Tr} \left(e^{-\beta \hat{H}_0} \right) = e^{-\beta F^{(0)}},$$

is the unperturbed partition function and $\langle \dots \rangle_0$ means a quantum and thermal average with the uncorrelated Boltzmann weight, namely

$$\langle \dots \rangle_0 \equiv \frac{1}{\mathcal{Z}_0} \text{Tr} \left(e^{-\beta \hat{H}_0} \dots \right).$$

In a perturbation expansion

$$\langle \hat{S}(\beta) \rangle_0 = \sum_{n=0} \langle \hat{S}^{(n)}(\beta) \rangle_0 = \sum_{n=0} S^{(n)} = 1 + S^{(1)} + S^{(2)} + \dots$$

Therefore

$$\begin{aligned} \mathcal{Z} &= e^{-\beta F^{(0)}} \left[1 - \beta F^{(1)} + \frac{1}{2} \beta^2 \left(F^{(1)} \right)^2 - \beta F^{(2)} + \dots \right] \\ &= e^{-\beta F^{(0)}} \left[1 + S^{(1)} + S^{(2)} + \dots \right], \end{aligned}$$

which leads to

$$F^{(1)} = -\frac{1}{\beta} S^{(1)} = -\frac{1}{\beta} \langle \hat{S}^{(1)}(\beta) \rangle_0 \quad (4.30)$$

$$F^{(2)} = -\frac{1}{\beta} S^{(2)} + \frac{1}{2} \beta \left(F^{(1)} \right)^2 = -\frac{1}{\beta} \langle \hat{S}^{(2)}(\beta) \rangle_0 + \frac{1}{2\beta} \left(\langle \hat{S}^{(1)}(\beta) \rangle_0 \right)^2. \quad (4.31)$$

Let us first consider (4.30). We need to calculate

$$\begin{aligned} \langle \hat{S}^{(1)}(\beta) \rangle_0 &= -\frac{1}{\mathcal{Z}_0} \text{Tr} \left[e^{-\beta \hat{H}_0} \int_0^\beta d\tau e^{\tau \hat{H}_0} \hat{V} e^{-\tau \hat{H}_0} \right] \\ &= -\frac{1}{\mathcal{Z}_0} \text{Tr} \left[e^{-\beta \hat{H}_0} \int_0^\beta d\tau \hat{V} \right] = -\beta \langle \hat{V} \rangle_0. \end{aligned} \quad (4.32)$$

Hence

$$F^{(1)} = \langle \hat{V} \rangle_0, \quad (4.33)$$

is the thermal average of the perturbation.

From the expression of $\hat{S}^{(2)}(\beta)$ one can easily show that

$$F^{(2)} = -\frac{1}{2\beta} \int_0^\beta d\tau_1 d\tau_2 \langle T_\tau \left[(\hat{V}(\tau_1) - \langle \hat{V} \rangle_0) (\hat{V}(\tau_2) - \langle \hat{V} \rangle_0) \right] \rangle_0. \quad (4.34)$$

Going up in perturbation theory, one finds that the generic $F^{(n)}$ is obtained by a cumulant expansion in powers of \hat{V} , namely an expansion in

$$\hat{V}(\tau) - \langle \hat{V} \rangle_0.$$

We want now to show that $F^{(2)} < 0$, which is the finite temperature analogue of the known result that second-order perturbation theory always decreases the ground state energy. Let us consider an hermitean operator $\hat{A}(\tau)$ such that $\langle \hat{A} \rangle_0 = 0$, a property shared also by $\hat{V}(\tau) - \langle \hat{V} \rangle_0$. Then

$$\begin{aligned} & \int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2 \text{Tr} \left[e^{-\beta \hat{H}_0} \hat{A}(\tau_1) \hat{A}(\tau_2) \right] \\ &= \sum_{n,m} \int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2 e^{-\beta \epsilon_n} e^{(\epsilon_n - \epsilon_m)(\tau_1 - \tau_2)} \left| \langle n | \hat{A} | m \rangle \right|^2 \\ &= \sum_{n,m} \left| \langle n | \hat{A} | m \rangle \right|^2 \left[\frac{e^{-\beta \epsilon_m} - e^{-\beta \epsilon_n}}{(\epsilon_n - \epsilon_m)^2} - \beta \frac{e^{-\beta \epsilon_n}}{\epsilon_n - \epsilon_m} \right]. \end{aligned}$$

Since the matrix element $\left| \langle n | \hat{A} | m \rangle \right|^2$ is even by interchanging $n \leftrightarrow m$, the first term in the square brackets, being odd, vanishes. The second term gives, after symmetrizing the sum $\sum_{n,m} f(n,m) = 1/2 \sum_{n,m} f(n,m) + f(m,n)$,

$$\frac{1}{2} \beta \sum_{n,m} \left| \langle n | \hat{A} | m \rangle \right|^2 \frac{e^{-\beta \epsilon_m} - e^{-\beta \epsilon_n}}{\epsilon_n - \epsilon_m},$$

which is always greater than zero.

By this result, one can write

$$F^{(2)} = -\frac{1}{2Z_0} \sum_{n,m} \left| \langle n | (\hat{V} - \langle \hat{V} \rangle_0) | m \rangle \right|^2 \frac{e^{-\beta \epsilon_m} - e^{-\beta \epsilon_n}}{\epsilon_n - \epsilon_m},$$

hence the desired result $F^{(2)} \leq 0$.

How do we use this property ? Let us consider the perturbed Hamiltonian

$$\hat{H}(\lambda) \equiv \hat{H}_0 + \lambda \hat{V}.$$

Then

$$F(\lambda) = F^{(0)} + \lambda F^{(1)} + \lambda^2 F^{(2)} + \dots,$$

where, as we showed, the curvature $F^{(2)} \leq 0$. Therefore in the interval $\lambda \in [0, 1]$, the function $F(\lambda)$ has a downwards curvature. This implies that in this interval

$$F(\lambda) \leq F^{(0)} + \lambda F^{(1)},$$

leading to the variational principle

$$F = F(\lambda = 1) \leq F^{(0)} + F^{(1)} = -\frac{1}{\beta} \ln \text{Tr} \left(e^{-\beta \hat{H}_0} \right) + \frac{1}{\text{Tr} \left(e^{-\beta \hat{H}_0} \right)} \text{Tr} \left(e^{-\beta \hat{H}_0} \hat{V} \right). \quad (4.35)$$

4.2.2 Variational approach at $T \neq 0$

Let us apply this finite temperature variational principle to our interacting problem.

The interacting Hamiltonian is, as usual,

$$\hat{H} = \sum_{\alpha\beta} t_{\alpha\beta} c_{\alpha}^{\dagger} c_{\beta} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} U_{\alpha\beta\gamma\delta} c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\gamma} c_{\delta}.$$

We define an unperturbed Hamiltonian

$$\hat{H}_0 = \sum_{\alpha\beta} (t_{\alpha\beta} + h_{\alpha\beta}) c_{\alpha}^{\dagger} c_{\beta},$$

which contains variational parameters $h_{\alpha\beta}$ [the similarity with (4.14) is not accidental, as we will show], so that

$$\hat{V} \equiv \hat{H} - \hat{H}_0 = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} U_{\alpha\beta\gamma\delta} c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\gamma} c_{\delta} - \sum_{\alpha\beta} h_{\alpha\beta} c_{\alpha}^{\dagger} c_{\beta}. \quad (4.36)$$

By the variational principle (4.35), we can get an upper bound to the true free energy by choosing the variational parameters $h_{\alpha\beta}$ which minimize the right hand side of (4.35). This is what we intend to do in the following.

Since \hat{H}_0 is quadratic in the fermionic fields, it can be diagonalized by some unitary transformation

$$c_{\alpha} = \sum_i \mathcal{U}_{\alpha i} c_i,$$

leading to

$$\hat{H}_0 = \sum_i \epsilon_i c_i^\dagger c_i.$$

Any many-body eigenstate of \hat{H}_0 , e.g. $|n\rangle$, with energy E_n , can be written as a single Slater determinant. The following property then holds

$$\begin{aligned} \langle c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta \rangle_0 &= \frac{1}{\mathcal{Z}_0} \sum_{ijkl} \mathcal{U}_{i\alpha}^\dagger \mathcal{U}_{j\beta}^\dagger \mathcal{U}_{\gamma k} \mathcal{U}_{\delta l} \text{Tr} \left(e^{-\beta \hat{H}_0} c_i^\dagger c_j^\dagger c_k c_l \right) \\ &= \frac{1}{\mathcal{Z}_0} \sum_{ijkl} \mathcal{U}_{i\alpha}^\dagger \mathcal{U}_{j\beta}^\dagger \mathcal{U}_{\gamma k} \mathcal{U}_{\delta l} \sum_n e^{-\beta E_n} \langle n | c_i^\dagger c_j^\dagger c_k c_l | n \rangle \\ &= \frac{1}{\mathcal{Z}_0} \sum_{ijkl} \mathcal{U}_{i\alpha}^\dagger \mathcal{U}_{j\beta}^\dagger \mathcal{U}_{\gamma k} \mathcal{U}_{\delta l} \sum_n e^{-\beta E_n} (\delta_{il} \delta_{jk} - \delta_{ik} \delta_{jl}) \langle n | c_i^\dagger c_i | n \rangle \langle n | c_j^\dagger c_j | n \rangle \\ &= \sum_{ijkl} \mathcal{U}_{i\alpha}^\dagger \mathcal{U}_{j\beta}^\dagger \mathcal{U}_{\gamma k} \mathcal{U}_{\delta l} (\delta_{il} \delta_{jk} - \delta_{ik} \delta_{jl}) f_i(T) f_j(T) \\ &= \langle c_\alpha^\dagger c_\delta \rangle_0 \langle c_\beta^\dagger c_\gamma \rangle_0 - \langle c_\alpha^\dagger c_\gamma \rangle_0 \langle c_\beta^\dagger c_\delta \rangle_0 \equiv \Delta_{\alpha\delta}(T) \Delta_{\beta\gamma}(T) - \Delta_{\alpha\gamma}(T) \Delta_{\beta\delta}(T), \end{aligned} \quad (4.37)$$

where

$$\mathcal{Z}_0 = \text{Tr} \left(e^{-\beta \hat{H}_0} \right) = \prod_i \left(1 + e^{-\beta \epsilon_i} \right),$$

is the partition function of \hat{H}_0 ,

$$f_i(T) = \frac{1}{1 + e^{\beta \epsilon_i}},$$

is the Fermi distribution function and we have introduced the thermal averages

$$\Delta_{\alpha\beta}(T) = \langle c_\alpha^\dagger c_\beta \rangle_0.$$

The previous result shows in a particular case the following general result

- the thermal average of a product of n creation and n annihilation operators with a bilinear Hamiltonian \hat{H}_0 , namely

$$\begin{aligned} \langle c_{i_1}^\dagger c_{i_2}^\dagger \dots c_{i_n}^\dagger c_{j_1} c_{j_2} \dots c_{j_n} \rangle_0 &= \frac{1}{\mathcal{Z}_0} \text{Tr} \left(e^{-\beta \hat{H}_0} c_{i_1}^\dagger c_{i_2}^\dagger \dots c_{i_n}^\dagger c_{j_1} c_{j_2} \dots c_{j_n} \right) \\ &= \sum_P (-1)^P \langle c_{i_1}^\dagger c_{j_{P_1}} \rangle_0 \langle c_{i_2}^\dagger c_{j_{P_2}} \rangle_0 \dots \langle c_{i_n}^\dagger c_{j_{P_n}} \rangle_0, \end{aligned} \quad (4.38)$$

where $(j_{P_1}, j_{P_2}, \dots, j_{P_n}) = P(j_1, j_2, \dots, j_n)$ is a permutation over the n j -indices and P is the order of the permutation. The most general case where the operators are not ordered in such a way that creation operators appear on the left can be straightforwardly derived

from the above result. Essentially one has to consider all possible contractions between a creation, c_i^\dagger , and an annihilation, c_j , operator. If the former is on the left of the latter, the contraction means

$$\langle c_i^\dagger c_j \rangle_0,$$

otherwise it means

$$\langle c_j c_i^\dagger \rangle_0.$$

The sign of a given product of contractions is plus or minus depending on the number of fermionic hops one has to do to bring each pair of operators to be contracted close together.

Coming back to our original scope, we need to solve the equation

$$\frac{\partial F^{(0)}}{\partial h_{\alpha\beta}} + \frac{\partial F^{(1)}}{\partial h_{\alpha\beta}} = 0.$$

Let us first consider the first term on the left-hand side. Since

$$F^{(0)} = -\frac{1}{\beta} \sum_i \ln \left(1 + e^{-\beta\epsilon_i} \right),$$

then

$$\frac{\partial F^{(0)}}{\partial h_{\alpha\beta}} = -\frac{1}{\beta} \sum_i \frac{e^{-\beta\epsilon_i}}{1 + e^{-\beta\epsilon_i}} \left(-\beta \frac{\partial \epsilon_i}{\partial h_{\alpha\beta}} \right) = \Delta_{\alpha\beta}(T). \quad (4.39)$$

This result derives from a general property, known as Hellmann-Feynmann theorem, which states the following.

- We consider a non-interacting Hamiltonian \hat{H}_0 with single particle eigenvalues ϵ_i and eigenfunctions $\phi_i(x)$, and a perturbed Hamiltonian

$$\hat{H}_0 + \delta\hat{H}_0 = \hat{H}_0 + \delta h_{\alpha\beta} c_\alpha^\dagger c_\beta,$$

with eigenvalues $\epsilon_i + \delta\epsilon_i$ and normalized eigenfunctions $N_i(\phi_i(x) + \delta\phi_i(x))$. Since $\langle \delta\phi_i | \phi_i \rangle + \langle \phi_i | \delta\phi_i \rangle = 0$, the normalization $N_i = 1 + O(\delta h^2)$, hence at linear order

$$\begin{aligned} \delta\epsilon_i &= \langle \phi_i + \delta\phi_i | \hat{H}_0 + \delta\hat{H}_0 | \phi_i + \delta\phi_i \rangle - \langle \phi_i | \hat{H}_0 | \phi_i \rangle \\ &= \langle \delta\phi_i | \hat{H}_0 | \phi_i \rangle + \langle \phi_i | \hat{H}_0 | \delta\phi_i \rangle + \langle \phi_i | \delta\hat{H}_0 | \phi_i \rangle = \epsilon_i (\langle \delta\phi_i | \phi_i \rangle + \langle \phi_i | \delta\phi_i \rangle) \\ &\quad + \delta h_{\alpha\beta} \langle \phi_i | c_\alpha^\dagger c_\beta | \phi_i \rangle = \delta h_{\alpha\beta} \langle \phi_i | c_\alpha^\dagger c_\beta | \phi_i \rangle. \end{aligned}$$

Therefore

$$\frac{\partial \epsilon_i}{\partial h_{\alpha\beta}} = \langle \phi_i | c_\alpha^\dagger c_\beta | \phi_i \rangle. \quad (4.40)$$

After inserting (4.40) into (4.39), one does obtain the right hand side.

By means of (4.37) we find that $F^{(1)}$ defined through (4.33) and (4.36) is given by

$$F^{(1)} = \langle \hat{V} \rangle_0 = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \Delta_{\alpha\beta}(T) \Delta_{\gamma\delta}(T) (U_{\alpha\gamma\delta\beta} - U_{\alpha\gamma\beta\delta}) - \sum_{\alpha\beta} h_{\alpha\beta} \Delta_{\alpha\beta}(T),$$

hence

$$\frac{\partial F^{(1)}}{\partial h_{\alpha\beta}} = -\Delta_{\alpha\beta}(T) - \sum_{\gamma\delta} h_{\gamma\delta} \frac{\partial \Delta_{\gamma\delta}}{\partial h_{\alpha\beta}} + \sum_{\gamma\delta\mu\nu} \frac{\partial \Delta_{\gamma\delta}}{\partial h_{\alpha\beta}} \Delta_{\mu\nu} (U_{\gamma\mu\nu\delta} - U_{\gamma\mu\delta\nu}). \quad (4.41)$$

The sum of (4.39) and (4.41) gives therefore

$$\sum_{\gamma\delta} \frac{\partial \Delta_{\gamma\delta}}{\partial h_{\alpha\beta}} \left[h_{\gamma\delta} - \sum_{\mu\nu} \Delta_{\mu\nu} (U_{\gamma\mu\nu\delta} - U_{\gamma\mu\delta\nu}) \right] = 0, \quad (4.42)$$

which should hold for every pair of indices $(\alpha\beta)$. The solution of this equation reads

$$h_{\gamma\delta} = \sum_{\mu\nu} \Delta_{\mu\nu}(T) (U_{\gamma\mu\nu\delta} - U_{\gamma\mu\delta\nu}) = \frac{1}{Z_0} \sum_{\mu\nu} (U_{\gamma\mu\nu\delta} - U_{\gamma\mu\delta\nu}) \text{Tr} \left(e^{-\beta \hat{H}_0} c_\mu^\dagger c_\nu \right). \quad (4.43)$$

Therefore the single particle Hamiltonian \hat{H}_0 which minimizes $F^{(0)} + F^{(1)}$, hence providing an upper bound to the exact free energy, is defined through variational parameters $h_{\alpha\beta}$ which have to be determined self-consistently through Eq. (4.43). Notice that this equation is just an extension of the Hartree-Fock Hamiltonian (4.14) at finite temperature, where the variational parameters have to correspond now to thermal averages and no more to ground state averages.

Finally notice that the Hartree-Fock Hamiltonian \hat{H}_0 represents non-interacting electrons in the presence of a *fictitious* external field which, through (4.43), is indeed the self-consistent field generated by the same electrons. This is the reason why the Hartree-Fock approximation is also called Mean-Field approximation.

4.3 Mean-Field approximation for bosons and superfluidity

The naïve Hartree-Fock approximation for interacting bosons, in the spirit of what we did for fermions, might be searching for the permanent of single-particle wavefunctions which has the lowest average value of the Hamiltonian. This is however not so easy in general because a permanent, unlike a Slater determinant, does not vanish if the single particle wavefunctions, out of which it is constructed, overlap each other. In addition, bosonic Hamiltonian fall into two different classes. The first includes models where the number of bosons is not a conserved quantity, e.g. phonons in solids. In this case a permanent, which is by definition a wavefunction for a fixed number of particles, is a very poor approximation for the actual ground state. The second class includes models where the number of bosons is conserved, as for instance models for liquid ^4He . Here however one has to face another problem, namely Bose condensation, and a single permanent is not expected to be a good approximation, too. In other words there is not a unique prescription for a simple and accurate mean-field approximation for bosons. In what follows we discuss an Hamiltonian for bosonic particles in the second class, i.e. which conserves the number of bosons, in the context of Bose superfluidity.

Let us consider the Hamiltonian for N bosonic particles

$$\mathcal{H} = \sum_{\mathbf{q}} \epsilon_{\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}} + \frac{1}{2V} \sum_{\mathbf{q} \mathbf{p} \mathbf{k}} U(\mathbf{q}) b_{\mathbf{p}}^\dagger b_{\mathbf{k}+\mathbf{q}}^\dagger b_{\mathbf{k}} b_{\mathbf{p}+\mathbf{q}}, \quad (4.44)$$

where the single particle energy

$$\epsilon_{\mathbf{q}} = \frac{\hbar^2 q^2}{2m}.$$

In the absence of interaction, the ground state is simply obtained by putting, i.e. condense, all N particles into the $\mathbf{q} = \mathbf{0}$ state. The interaction is going to mix this state with excited states, by moving particles from $\mathbf{q} = \mathbf{0}$ to $\mathbf{q} \neq \mathbf{0}$. First of all let us rewrite the interaction term as

$$\begin{aligned} \frac{1}{2V} \sum_{\mathbf{q} \mathbf{p} \mathbf{k}} U(\mathbf{q}) b_{\mathbf{p}}^\dagger b_{\mathbf{k}+\mathbf{q}}^\dagger b_{\mathbf{k}} b_{\mathbf{p}+\mathbf{q}} &= \frac{U(\mathbf{0})}{2V} \sum_{\mathbf{p} \mathbf{k}} b_{\mathbf{p}}^\dagger b_{\mathbf{k}}^\dagger b_{\mathbf{k}} b_{\mathbf{p}} \\ &+ \frac{1}{2V} \sum_{\mathbf{q} \neq \mathbf{0}} \sum_{\mathbf{p} \mathbf{k}} U(\mathbf{q}) b_{\mathbf{p}}^\dagger b_{\mathbf{k}+\mathbf{q}}^\dagger b_{\mathbf{k}} b_{\mathbf{p}+\mathbf{q}} \\ &= \frac{U(\mathbf{0})}{2V} N(N-1) + \frac{1}{2V} \sum_{\mathbf{q} \neq \mathbf{0}} \sum_{\mathbf{p} \mathbf{k}} U(\mathbf{q}) b_{\mathbf{p}}^\dagger b_{\mathbf{k}+\mathbf{q}}^\dagger b_{\mathbf{k}} b_{\mathbf{p}+\mathbf{q}}, \end{aligned}$$

which shows that the $\mathbf{q} = \mathbf{0}$ component of the interaction is just a constant since the number of bosons is conserved. Therefore, discarding this constant, the Hamiltonian can be written as

$$\mathcal{H} = \sum_{\mathbf{q}} \epsilon_{\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}} + \frac{1}{2V} \sum_{\mathbf{q} \neq \mathbf{0}} \sum_{\mathbf{p} \mathbf{k}} U(\mathbf{q}) b_{\mathbf{p}}^\dagger b_{\mathbf{k}+\mathbf{q}}^\dagger b_{\mathbf{k}} b_{\mathbf{p}+\mathbf{q}}, \quad (4.45)$$

We will assume that the interaction is weak enough that the actual ground state is a slight modification of the state where all bosons condense into the state $\mathbf{q} = \mathbf{0}$.

Let us consider the following unitary transformation acting on the $\mathbf{q} = \mathbf{0}$ bosons:

$$\mathcal{U} = \exp \left[\sqrt{N_0} \left(b_{\mathbf{0}}^\dagger - b_{\mathbf{0}} \right) \right].$$

It follows that

$$\mathcal{U}^\dagger b_{\mathbf{0}} \mathcal{U} = b_{\mathbf{0}} + \sqrt{N_0}, \quad \mathcal{U}^\dagger b_{\mathbf{0}}^\dagger \mathcal{U} = b_{\mathbf{0}}^\dagger + \sqrt{N_0}.$$

Therefore, if we consider a so-called coherent state

$$|\tilde{0}\rangle \equiv \mathcal{U} |0\rangle,$$

then

$$\begin{aligned} \langle \tilde{0} | b_{\mathbf{0}}^\dagger b_{\mathbf{0}} | \tilde{0} \rangle &= N_0, \\ \langle \tilde{0} | b_{\mathbf{0}}^\dagger b_{\mathbf{0}}^\dagger | \tilde{0} \rangle &= \langle \tilde{0} | b_{\mathbf{0}} b_{\mathbf{0}} | \tilde{0} \rangle = N_0. \end{aligned}$$

In other words $|\tilde{0}\rangle$ contains an average number N_0 of bosons at $\mathbf{q} = \mathbf{0}$, but, at the meantime, it is not eigenstate of $b_{\mathbf{0}}^\dagger b_{\mathbf{0}}$. On the other hand, the number fluctuation behaves as

$$\Delta N^2 = \langle \tilde{0} | \left(b_{\mathbf{0}}^\dagger b_{\mathbf{0}} - N_0 \right)^2 | \tilde{0} \rangle = N_0,$$

hence, for large N_0 , $\Delta N/N_0 \rightarrow 0$. These properties suggest that $|\tilde{0}\rangle$ might be a good representation of a state in which bosons condense into the zero-momentum state but fluctuations of charge from $\mathbf{q} = \mathbf{0}$ to $\mathbf{q} \neq \mathbf{0}$ are still possible. Therefore, let us assume as a variational wavefunction

$$|\Psi\rangle = |\tilde{0}\rangle |\Phi_{\mathbf{q} \neq \mathbf{0}}\rangle,$$

where $|\Phi_{\mathbf{q} \neq \mathbf{0}}\rangle$ includes non-zero momentum bosons, supplemented by the constraint

$$\langle \Psi | b_{\mathbf{0}}^\dagger b_{\mathbf{0}} + \sum_{\mathbf{q} \neq \mathbf{0}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}} | \Psi \rangle = N_0 + \sum_{\mathbf{q} \neq \mathbf{0}} \langle b_{\mathbf{q}}^\dagger b_{\mathbf{q}} \rangle = N. \quad (4.46)$$

As we pointed out, such a variational wavefunction should be a faithful representation of the ground state provided

$$N - N_0 \ll N, \quad (4.47)$$

which we are going to assume in what follows and check *a posteriori*.

The average of the Hamiltonian over $|\tilde{0}\rangle$ leads to an effective Hamiltonian for the $\mathbf{q} \neq \mathbf{0}$ bosons which reads

$$\mathcal{H}_{eff} = \sum_{\mathbf{q} \neq \mathbf{0}} \epsilon_{\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}} + \frac{N_0}{V} \sum_{\mathbf{q} \neq \mathbf{0}} U(\mathbf{q}) b_{\mathbf{q}}^\dagger b_{\mathbf{q}} + \frac{N_0}{2V} \sum_{\mathbf{q} \neq \mathbf{0}} U(\mathbf{q}) \left(b_{\mathbf{q}}^\dagger b_{-\mathbf{q}}^\dagger + b_{-\mathbf{q}} b_{\mathbf{q}} \right)$$

$$+ \frac{\sqrt{N_0}}{V} \sum_{\mathbf{q} \neq \mathbf{0}} U(\mathbf{q}) \left(b_{\mathbf{p}}^\dagger b_{\mathbf{q}}^\dagger b_{\mathbf{p}+\mathbf{q}} + b_{\mathbf{p}+\mathbf{q}}^\dagger b_{\mathbf{q}} b_{\mathbf{p}} \right) + \frac{1}{2V} \sum_{\mathbf{q} \neq \mathbf{0}} \sum_{\mathbf{k} \neq \mathbf{0}} U(\mathbf{q}) b_{\mathbf{p}}^\dagger b_{\mathbf{k}+\mathbf{q}}^\dagger b_{\mathbf{k}} b_{\mathbf{p}+\mathbf{q}}.$$

Notice that the first two interaction terms are proportional to $N_0(N - N_0)$ while the last two can be shown to be of order $(N - N_0)^2$. Therefore, in view of the assumption (4.47), we are going to start from the Hamiltonian

$$\begin{aligned} \mathcal{H}_0 = & \sum_{\mathbf{q} \neq \mathbf{0}} \epsilon_{\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}} + \frac{N_0}{V} \sum_{\mathbf{q} \neq \mathbf{0}} U(\mathbf{q}) b_{\mathbf{q}}^\dagger b_{\mathbf{q}} \\ & + \frac{N_0}{2V} \sum_{\mathbf{q} \neq \mathbf{0}} U(\mathbf{q}) \left(b_{\mathbf{q}}^\dagger b_{-\mathbf{q}}^\dagger + b_{-\mathbf{q}} b_{\mathbf{q}} \right), \end{aligned} \quad (4.48)$$

and eventually treat as a perturbation

$$\begin{aligned} \mathcal{H}_{int} = & \frac{\sqrt{N_0}}{V} \sum_{\mathbf{q} \neq \mathbf{0}} U(\mathbf{q}) \left(b_{\mathbf{p}}^\dagger b_{\mathbf{q}}^\dagger b_{\mathbf{p}+\mathbf{q}} + b_{\mathbf{p}+\mathbf{q}}^\dagger b_{\mathbf{q}} b_{\mathbf{p}} \right) \\ & + \frac{1}{2V} \sum_{\mathbf{q} \neq \mathbf{0}} \sum_{\mathbf{k} \neq \mathbf{0}} U(\mathbf{q}) b_{\mathbf{p}}^\dagger b_{\mathbf{k}+\mathbf{q}}^\dagger b_{\mathbf{k}} b_{\mathbf{p}+\mathbf{q}}. \end{aligned} \quad (4.49)$$

Let us introduce conjugate variables through

$$\begin{aligned} x_{\mathbf{q}} &= \sqrt{\frac{1}{2}} \left(b_{\mathbf{q}} + b_{-\mathbf{q}}^\dagger \right), \\ p_{\mathbf{q}} &= -i \sqrt{\frac{1}{2}} \left(b_{\mathbf{q}} - b_{-\mathbf{q}}^\dagger \right), \end{aligned}$$

which satisfy

$$[x_{\mathbf{p}}, p_{-\mathbf{k}}] = i \delta_{\mathbf{p}, \mathbf{k}}.$$

In terms of these variables (4.48) becomes

$$\mathcal{H}_0 = \sum_{\mathbf{q} \neq \mathbf{0}} \frac{1}{2} \left(\epsilon_{\mathbf{q}} + n_0 U(\mathbf{q}) \right) \left(x_{\mathbf{q}} x_{-\mathbf{q}} + p_{\mathbf{q}} p_{-\mathbf{q}} - 1 \right) + \frac{1}{2} n_0 U(\mathbf{q}) \left(x_{\mathbf{q}} x_{-\mathbf{q}} - p_{\mathbf{q}} p_{-\mathbf{q}} \right), \quad (4.50)$$

where $n_0 = N_0/V$, which can be diagonalized by the canonical transformation

$$x_{\mathbf{q}} \rightarrow \sqrt{K_{\mathbf{q}}} x_{\mathbf{q}}, \quad p_{\mathbf{q}} \rightarrow \sqrt{\frac{1}{K_{\mathbf{q}}}} p_{\mathbf{q}},$$

with

$$K_{\mathbf{q}}^2 = \frac{\epsilon_{\mathbf{q}}}{\epsilon_{\mathbf{q}} + 2n_0 U(\mathbf{q})}, \quad (4.51)$$

leading to

$$\mathcal{H}_0 = -\frac{1}{2} \sum_{\mathbf{q} \neq \mathbf{0}} (\epsilon_{\mathbf{q}} + n_0 U(\mathbf{q})) + \frac{1}{2} \sum_{\mathbf{q} \neq \mathbf{0}} \omega_{\mathbf{q}} (x_{\mathbf{q}} x_{-\mathbf{q}} + p_{\mathbf{q}} p_{-\mathbf{q}}), \quad (4.52)$$

with the frequency

$$\omega_{\mathbf{q}} = \sqrt{\epsilon_{\mathbf{q}} (\epsilon_{\mathbf{q}} + 2n_0 U(\mathbf{q}))}. \quad (4.53)$$

For small \mathbf{q} , if $U(\mathbf{q} \rightarrow \mathbf{0})$ is finite,

$$\omega_{\mathbf{q}} \rightarrow \hbar q \sqrt{\frac{n_0 U(\mathbf{0})}{m}} = s q,$$

thus showing that the long wavelength excitations describe acoustic phonons, which are actually

the Goldstone modes since the wave-function explicitly breaks gauge invariance.¹

Let us go back to the Hamiltonian (4.52). We notice that

$$\langle b_{\mathbf{q}}^\dagger b_{\mathbf{q}} \rangle = \frac{1}{2} \langle x_{\mathbf{q}} x_{-\mathbf{q}} + p_{\mathbf{q}} p_{-\mathbf{q}} - 1 \rangle = \frac{1}{4} \left(K_{\mathbf{q}} + \frac{1}{K_{\mathbf{q}}} - 2 \right).$$

Therefore the constraint (4.46) implies the following self-consistency equation for n_0

$$\frac{N}{V} = n_0 + \frac{1}{4V} \sum_{\mathbf{q} \neq 0} \left(K_{\mathbf{q}} + \frac{1}{K_{\mathbf{q}}} - 2 \right).$$

Since $K_{\mathbf{q}} \sim q$ for small q 's, this self-consistency equation can be always solved but in one dimension, where the summation diverges. Once more this tells us that a continuous symmetry,

¹Indeed the original Hamiltonian has a gauge symmetry, namely is invariant upon the transformation

$$b_{\mathbf{q}} \rightarrow e^{i\phi} b_{\mathbf{q}}, \quad b_{\mathbf{q}}^\dagger \rightarrow e^{-i\phi} b_{\mathbf{q}}^\dagger,$$

generated by the unitary operator

$$\mathcal{T}_\phi = \exp \left(i\phi \sum_{\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}} \right).$$

As usual, this implies that, given a generic normalized eigenstate $|\Psi_n\rangle$ with eigenvalue E_n , the state $\mathcal{T}_\phi |\Psi_n\rangle$ is also a normalized eigenstate with the same eigenvalue. There are two possible cases: either $\mathcal{T}_\phi |\Psi_n\rangle$ is, for all ϕ 's, the same $|\Psi_n\rangle$ apart from a phase factor, namely

$$|\langle \Psi_n | \mathcal{T}_\phi | \Psi_n \rangle| = 1,$$

or it is different, i.e.

$$|\langle \Psi_n | \mathcal{T}_\phi | \Psi_n \rangle| < 1.$$

The former case means that $|\Psi_n\rangle$ is invariant under a gauge transformation, while the latter case implies that it is not, hence that the eigenvalue E_n is degenerate. Let us suppose that our variational wave-function is indeed a good approximation of the actual ground state $|\Psi_0\rangle$, which is therefore also characterized by a finite value of

$$\langle \Psi_0 | b_0 | \Psi_0 \rangle \neq 0.$$

On the other hand

$$\langle \Psi_0 | b_0 | \Psi_0 \rangle = e^{-i\phi} \langle \Psi_0 | \mathcal{T}_\phi^\dagger b_0 \mathcal{T}_\phi | \Psi_0 \rangle.$$

If $|\Psi_0\rangle$ is not degenerate, then $\mathcal{T}_\phi |\Psi_0\rangle = e^{i\gamma} |\Psi_0\rangle$, with γ a real number, hence we would get

$$\langle \Psi_0 | b_0 | \Psi_0 \rangle = e^{-i\phi} \langle \Psi_0 | b_0 | \Psi_0 \rangle.$$

This equality, being true for any ϕ , would necessarily imply that $\langle \Psi_0 | b_0 | \Psi_0 \rangle = 0$. Therefore, in order for this average value to be finite, the ground state has to be degenerate and generically not gauge invariant. Notice that in principle, given one of the degenerate ground states, say $|\Psi_0\rangle$, one can always construct a gauge invariant combination by

$$|\tilde{\Psi}_0\rangle = \int d\phi \mathcal{T}_\phi |\Psi_0\rangle.$$

Yet, all other orthogonal combinations will remain not gauge invariant.

as the gauge symmetry is, can not be broken spontaneously in one dimension. Notice in addition that the summation vanishes when $U(\mathbf{q}) \rightarrow 0$, namely when $K_{\mathbf{q}} \rightarrow 1$, so that, for sufficiently small interaction, indeed $N - N_0 \ll N$, thus justifying our approximation.

4.3.1 Superfluid properties of the gauge symmetry breaking wavefunction

Let us uncover now some interesting properties of the variational wavefunction. By definition the Fourier transform of the current operator is

$$\mathbf{J}_{\mathbf{q}} = \frac{\hbar}{m} \sum_{\mathbf{k}} \left(\mathbf{k} + \frac{\mathbf{q}}{2} \right) b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}+\mathbf{q}}. \quad (4.54)$$

In the spirit of our approximation, the leading term of the current is obtained when either $\mathbf{k} = \mathbf{0}$ or $\mathbf{k} + \mathbf{q} = \mathbf{0}$, leading to

$$\mathbf{J}_{\mathbf{q}} \simeq \sqrt{N_0} \frac{\hbar \mathbf{q}}{2m} \left(b_{\mathbf{q}} - b_{-\mathbf{q}}^{\dagger} \right) = i \sqrt{2N_0} \frac{\hbar \mathbf{q}}{2m} p_{\mathbf{q}}. \quad (4.55)$$

In other words the current is purely longitudinal, i.e. $\mathbf{q} \wedge \mathbf{J}_{\mathbf{q}} = 0$. Let us check whether (4.55) is compatible, within the same scheme, with the continuity equation

$$i\hbar \frac{\partial \rho_{\mathbf{q}}}{\partial t} = [\rho_{\mathbf{q}}, \mathcal{H}_0] = \mathbf{q} \cdot \mathbf{J}_{\mathbf{q}}.$$

The density operator at leading order is

$$\rho_{\mathbf{q}} = \sum_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}+\mathbf{q}} \simeq \sqrt{N_0} \left(b_{\mathbf{q}} + b_{-\mathbf{q}}^{\dagger} \right) = \sqrt{2N_0} x_{\mathbf{q}},$$

and one readily verifies that its commutation with the Hamiltonian \mathcal{H}_0 indeed reproduces $\mathbf{q} \cdot \mathbf{J}_{\mathbf{q}}$, with the current given by (4.55).

Non-Classical Rotational Inertia

What is the consequence of a purely longitudinal current? Let us suppose that our system of N bosons with mass m is enclosed in a cylindrical annulus, initially at rest, with internal radius R and thickness d , with $d/R \ll 1$. At a given time the cylinder is made moving around its axis, assumed to be the z -axis, with constant angular velocity ω . A normal liquid would be dragged by the walls of the cylinder and rotate at the same angular velocity ω . Neglecting the mass of the cylinder, the energy change at equilibrium due to rotation would simply be at leading order in ω

$$\mathcal{E}(\omega) - \mathcal{E}(0) = \frac{1}{2} I_0 \omega^2,$$

where the classical moment of inertia $I_0 \simeq mNR^2$ if $d \ll R$. Let us consider what happens in our Bose-condensed fluid. The Schrödinger equation describing the system reads

$$\begin{aligned} i\hbar \frac{d\Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N; t)}{dt} &= -\frac{\hbar^2}{2m} \sum_{i=1}^N \nabla_i^2 \Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N; t) \\ &\quad + \frac{1}{2} \sum_{i \neq j} U(\mathbf{x}_i - \mathbf{x}_j) \Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N; t) \\ &\quad + \sum_{i=1}^N V(\mathbf{x}_i; t) \Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N; t), \end{aligned}$$

where $V(\mathbf{x}; t)$ represents the coupling of a boson with the rotating walls of the cylinder, hence it is explicitly time-dependent. We use cylindrical coordinates, so that the position of particle i is

$$\mathbf{x}_i = (r \cos \theta, r \sin \theta, z) \equiv \mathbf{r}_i + z_i \mathbf{z},$$

where \mathbf{z} is the unit vector in the z -direction. Let us consider the following transformation on the planar coordinate

$$\boldsymbol{\rho}_i(t) = \cos \omega t \mathbf{r}_i + \sin \omega t \mathbf{r}_i \wedge \mathbf{z}, \quad (4.56)$$

which corresponds to a reference frame in which the cylinder is at rest. In this frame

$$V(\mathbf{x}; t) = V(\mathbf{r}, z; t) = V(\boldsymbol{\rho}(t), z),$$

namely the explicit time-dependence of the interaction with the wall is being transformed into an implicit one via the time-dependence of $\boldsymbol{\rho}(t)$. We rewrite the many-body wavefunction in terms of the new variables, i.e.

$$\Psi((\mathbf{r}_1, z_1), (\mathbf{r}_2, z_2), \dots, (\mathbf{r}_N, z_N); t) = \Psi((\boldsymbol{\rho}_1, z_1), (\boldsymbol{\rho}_2, z_2), \dots, (\boldsymbol{\rho}_N, z_N); t).$$

In this representation the wavefunction depends both explicitly upon time and also implicitly, via the coordinates $\boldsymbol{\rho}_i$'s. Therefore

$$\begin{aligned} i\hbar \frac{d\Psi((\mathbf{r}_1, z_1), (\mathbf{r}_2, z_2), \dots, (\mathbf{r}_N, z_N); t)}{dt} &= i\hbar \frac{\partial \Psi((\boldsymbol{\rho}_1, z_1), (\boldsymbol{\rho}_2, z_2), \dots, (\boldsymbol{\rho}_N, z_N); t)}{\partial t} \\ &\quad + i\hbar \sum_{i=1}^N \frac{\partial \boldsymbol{\rho}_i}{\partial t} \cdot \nabla_i \Psi((\boldsymbol{\rho}_1, z_1), (\boldsymbol{\rho}_2, z_2), \dots, (\boldsymbol{\rho}_N, z_N); t) \\ &= i\hbar \frac{\partial \Psi((\boldsymbol{\rho}_1, z_1), (\boldsymbol{\rho}_2, z_2), \dots, (\boldsymbol{\rho}_N, z_N); t)}{\partial t} \\ &\quad + i\hbar \omega \sum_{i=1}^N \boldsymbol{\rho}_i \wedge \mathbf{z} \cdot \nabla_i \Psi((\boldsymbol{\rho}_1, z_1), (\boldsymbol{\rho}_2, z_2), \dots, (\boldsymbol{\rho}_N, z_N); t) \end{aligned}$$

$$= i\hbar \frac{\partial \Psi((\rho_1, z_1), (\rho_2, z_2), \dots, (\rho_N, z_N); t)}{\partial t} - m\omega \sum_{i=1}^N \rho_i \wedge \mathbf{z} \cdot \mathbf{J}_i \Psi((\rho_1, z_1), (\rho_2, z_2), \dots, (\rho_N, z_N); t),$$

where ∇_i is assumed to act on the new coordinate basis and by definition the current operator is

$$\mathbf{J}_i = -\frac{i\hbar}{m} \nabla_i.$$

One can readily verify that the Laplacian is invariant upon the transformation (4.56), hence the Schrödinger equation becomes

$$\begin{aligned} i\hbar \frac{\partial \Psi}{\partial t} &= \sum_{i=1}^N \left(-\frac{\hbar^2}{2m} \nabla_i^2 + m\omega \rho_i \wedge \mathbf{z} \cdot \mathbf{J}_i \right) \Psi \\ &\quad + \frac{1}{2} \sum_{ij} U(\rho_i - \rho_j, z_i - z_j) \Psi + \sum_{i=1}^N V(\rho_i, z_i) \Psi. \end{aligned} \quad (4.57)$$

Unlike in the original representation, this equation is not explicitly time-dependent, hence it admits stationary solutions

$$\Psi((\rho_1, z_1), (\rho_2, z_2), \dots, (\rho_N, z_N); t) = e^{iE(\omega)t/\hbar} \Psi((\rho_1, z_1), (\rho_2, z_2), \dots, (\rho_N, z_N)).$$

The minimum energy $E(\omega)$ corresponds to the equilibrium condition.²

It is important to recognize that the actual average value of the Hamiltonian is not $E(\omega)$ but³

$$\begin{aligned} \mathcal{E}(\omega) &= \int \prod_i d\mathbf{r}_i dz_i \Psi((\mathbf{r}_1, z_1), (\mathbf{r}_2, z_2), \dots, (\mathbf{r}_N, z_N); t)^* i\hbar \frac{d}{dt} \Psi((\mathbf{r}_1, z_1), (\mathbf{r}_2, z_2), \dots, (\mathbf{r}_N, z_N); t) \\ &= \int \prod_i d\rho_i dz_i \Psi((\rho_1, z_1), (\rho_2, z_2), \dots, (\rho_N, z_N); t)^* \left(i\hbar \frac{\partial}{\partial t} - m\omega \sum_j \rho_j \wedge \mathbf{z} \cdot \mathbf{J}_j \right) \\ &\quad \Psi((\rho_1, z_1), (\rho_2, z_2), \dots, (\rho_N, z_N); t) \\ &= \int \prod_i d\rho_i dz_i \Psi((\rho_1, z_1), (\rho_2, z_2), \dots, (\rho_N, z_N))^* \left(E(\omega) - m\omega \sum_j \rho_j \wedge \mathbf{z} \cdot \mathbf{J}_j \right) \end{aligned}$$

²Notice that the equilibrium condition corresponds to the minimum energy in a reference frame in which the cylinder is at rest. Indeed, it is only in such a reference frame that the walls of the cylinder can stop transferring energy to the liquid.

³The jacobian of the transformation (4.56) is unity.

$$\begin{aligned} & \Psi((\rho_1, z_1), (\rho_2, z_2), \dots, (\rho_N, z_N)) \\ = & E(\omega) - m\omega \sum_i \langle \rho_i \wedge \mathbf{z} \cdot \mathbf{J}_i \rangle. \end{aligned} \quad (4.58)$$

Therefore, in order to evaluate $\mathcal{E}(\omega)$ we first need to study the model described by the Hamiltonian in second quantization

$$\begin{aligned} \mathcal{H} = & \int d\mathbf{x} \Psi(\mathbf{x})^\dagger \left[-\frac{\hbar}{2m} \nabla^2 + \mathbf{A}(\mathbf{x}) \cdot \mathbf{J} + V(\mathbf{x}) \right] \Psi(\mathbf{x}) \\ & + \frac{1}{2} \int d\mathbf{x} d\mathbf{y} \Psi(\mathbf{x})^\dagger \Psi(\mathbf{y})^\dagger U(\mathbf{x} - \mathbf{y}) \Psi(\mathbf{y}) \Psi(\mathbf{x}), \end{aligned}$$

with

$$\mathbf{A}(\mathbf{x}) = m\omega \mathbf{x} \wedge \mathbf{z} = m\omega (y, -x, 0), \quad (4.59)$$

playing the role of a vector potential coupled to the current operator

$$\mathbf{J} = -i \frac{\hbar}{m} \nabla.$$

We notice that

$$\nabla \cdot \mathbf{A}(\mathbf{x}) = 0,$$

namely the vector potential is purely transverse. If we assume that the liquid is homogeneous, then, as we previously proved, the leading component of the current operator is purely longitudinal, hence the net effect of the transverse perturbation to the system is negligible. Therefore, within our approximation, $E(\omega) \simeq E(0)$ does not depend upon ω . Analogously

$$\langle \mathbf{J} \cdot \mathbf{A} \rangle \simeq 0,$$

implying that also $\mathcal{E}(\omega) \simeq E(0)$ is ω -independent. In other words, the actual moment of inertia is zero, i.e. the quantum liquid can not be made moving by rotating the cylinder, so called Non-Classical Rotational Inertia (NCRI).

In reality the situation may be more complex. Indeed, if the frequency of rotation exceed a critical value ω_{c1} , the lowest energy configuration ceases to be homogeneous, as we assumed so far, because line defects, so-called vortex lines, appear. It is however not our scope here to discuss vortices.

Superfluid flow

Let us consider another hypothetical experiment in which the bosonic fluid is made moving inside a capillary with constant velocity \mathbf{v} parallel to the walls of the capillary. A normal fluid, due to the friction, will be slowed down by the walls. Let us consider instead what happens with our

Bose-condensed fluid. In the reference frame in which the fluid is at rest, hence the capillary moves, we may expect that energy is transferred from the moving walls to the fluid leading to creation of excitations. Let us assume that an excitation of momentum \mathbf{q} and energy $\omega_{\mathbf{q}}$ is present. In the original reference frame in which the capillary is at rest, the actual energy is, by a Galilean transformation,

$$\mathcal{E}(\mathbf{q}) = \omega_{\mathbf{q}} + \mathbf{v} \cdot \mathbf{q} + \frac{Nm v^2}{2}.$$

As we said the equilibrium condition corresponds to the minimum of $\mathcal{E}(\mathbf{q})$, which is obtained by a momentum antiparallel to \mathbf{v} , i.e. $\mathbf{q} \cdot \mathbf{v} = -q v$. In this case

$$\mathcal{E}(\mathbf{q}) = \omega_{\mathbf{q}} - v q + \frac{Nm v^2}{2}.$$

It is clear that it is advantageous to create excitations only if

$$v \geq \frac{\omega_{\mathbf{q}}}{q}. \quad (4.60)$$

This is the famous Landau criterium for superfluidity. It tells us that the fluid can flow without resistance through a capillary, so-called **superfluidity**, for velocities below a critical one v_c defined by

$$v_c = \lim_{q \rightarrow 0} \frac{\omega_{\mathbf{q}}}{q}.$$

From our previous analysis it derives that $v_c = s$, the velocity of the acoustic phonons in the liquid. We notice that the interaction among the particles is essential for superfluidity. Indeed an ideal non-interacting Bose gas with dispersion $\hbar^2 q^2 / 2m$ has

$$v_c = \lim_{q \rightarrow 0} \frac{1}{q} \frac{\hbar^2 q^2}{2m} = 0,$$

hence it is not superfluid.

4.4 Time-dependent Hartree-Fock approximation for fermions

Let us move back to the Hartree-Fock approximation for fermions, and suppose to have solved the time-independent Hartree-Fock approximation, namely to have found a set of single particle wave-functions $\phi_i(x)$'s which diagonalize

$$t_{ij} + \sum_{k=1}^N U_{ikkj} - U_{ikjk} = \epsilon_i \delta_{ij}. \quad (4.61)$$

The Hartree-Fock wave-function is the Slater determinant

$$|\Phi_{HF}\rangle = \prod_{i=1}^N c_i^\dagger |0\rangle, \quad (4.62)$$

where c_i^\dagger creates a fermion in state ϕ_i . The original Hamiltonian in the Hartree-Fock basis is given by

$$\hat{H} = \sum_{ij} t_{ij} c_i^\dagger c_j + \frac{1}{2} \sum_{ijkl} U_{ijkl} c_i^\dagger c_j^\dagger c_k c_l. \quad (4.63)$$

Let us suppose to perturb the Hamiltonian by a time-dependent perturbation

$$\hat{V} = \sum_{ij} V_{ij}(t) c_i^\dagger c_j, \quad (4.64)$$

and let us study the response of the system to linear order. Therefore the full Hamiltonian $\hat{H}(t) = \hat{H} + \hat{V}(t)$ is time-dependent and the variational principle now concerns the time dependent Shrödinger equation. Namely **we will search within the subspace of time-dependent Slater determinants for a $|\Phi_{HF}(t)\rangle$ which satisfies**

$$\delta \left[\frac{\langle \Phi_{HF}(t) | i\hbar \frac{\partial}{\partial t} - \hat{H}(t) | \Phi_{HF}(t) \rangle}{\langle \Phi_{HF}(t) | \Phi_{HF}(t) \rangle} \right] = 0. \quad (4.65)$$

We assume that the time-dependent Slater determinant is build up by N single particle normalized wave-functions $\phi_\alpha(x, t)$. By analogy with the conventional derivation of the time-independent Hartree-Fock equations, one finds that

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \phi_\alpha(x, t) &= [T(x, p) + V(x, p, t)] \phi_\alpha(x, t) \\ &+ \sum_{\beta=1}^N \int dy U(x, y) [|\phi_\beta(y, t)|^2 \phi_\alpha(x, t) - \phi_\beta(y, t)^* \phi_\alpha(y, t) \phi_\beta(x, t)], \end{aligned} \quad (4.66)$$

where $T(x, p)$ is the single-particle term of the Hamiltonian, $V(x, p, t)$ the perturbation and $U(x, y)$ the interaction. We assume that the $\phi_\alpha(x, t)$'s are related to the $\phi_i(x)$'s by the time-dependent unitary transformation

$$\phi_\alpha(x, t) = \sum_i \mathcal{U}_{i\alpha}(t) \phi_i(x),$$

where

$$\mathcal{U}_{i\alpha}(t) = \int dx \phi_i(x)^* \phi_\alpha(x, t).$$

In terms of the matrix elements, the time-dependent equations (4.66) read

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \mathcal{U}_{i\alpha}(t) &= \sum_j [t_{ij} + V_{ij}(t)] \mathcal{U}_{j\alpha}(t) \\ &\quad + \sum_{\beta=1}^N \sum_{jkl} \mathcal{U}_{k\beta}(t)^* \mathcal{U}_{l\beta}(t) \mathcal{U}_{j\alpha}(t) [U_{iklj} - U_{ikjl}] . \end{aligned} \quad (4.67)$$

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \mathcal{U}_{i\alpha}(t)^* &= - \sum_j [t_{ji} + V_{ji}(t)] \mathcal{U}_{j\alpha}(t)^* \\ &\quad - \sum_{\beta=1}^N \sum_{jkl} \mathcal{U}_{k\beta}(t) \mathcal{U}_{l\beta}(t)^* \mathcal{U}_{j\alpha}(t)^* [U_{jlkj} - U_{ljkj}] . \end{aligned} \quad (4.68)$$

The time-dependent Hartree-Fock wave-function is identified by the matrix elements

$$\Delta_{ij}(t) = \langle \Phi_{HF}(t) | c_i^\dagger c_j | \Phi_{HF}(t) \rangle = \sum_{\alpha=1}^N \mathcal{U}_{i\alpha}(t)^* \mathcal{U}_{j\alpha}(t) , \quad (4.69)$$

which, calculated with the time-independent wave-function (4.62) are simply

$$\Delta_{ij}^{(0)} = \delta_{ij} n_i, \quad (4.70)$$

with $n_i = 1$ if $i \leq N$ and $n_i = 0$ otherwise. Through (4.67), (4.68) and (4.69) we obtain the following equations for the Δ_{ij} 's:

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \Delta_{ij}(t) &= \sum_k -[t_{ki} + V_{ki}(t)] \Delta_{kj}(t) + [t_{jk} + V_{jk}(t)] \Delta_{ik}(t) \\ &\quad + \sum_{klm} -\Delta_{kl}(t) \Delta_{mj}(t) [U_{mkli} - U_{kmlj}] \\ &\quad + \Delta_{il}(t) \Delta_{km}(t) [U_{jkml} - U_{jklm}] . \end{aligned} \quad (4.71)$$

We solve the above equation up to first order in the perturbation V . One can easily check that the zero order time-independent term is indeed given by (4.70). The first order terms satisfy the equation

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \Delta_{ij}^{(1)}(t) &= \sum_k - \left[t_{ki} + \sum_{m=1}^N (U_{kmmi} - U_{mkmi}) \right] \Delta_{kj}^{(1)}(t) \\ &\quad + \sum_k \left[t_{jk} + \sum_{m=1}^n (U_{jmmp} - U_{jmkp}) \right] \Delta_{ik}^{(1)}(t) \\ &\quad + (n_i - n_j) \sum_{lm} \Delta_{ml}^{(1)}(t) [U_{jmli} - U_{jmlp}] + V_{ji}(t) (n_i - n_j). \end{aligned} \quad (4.72)$$

Through Eq. (4.61) we finally obtain

$$\begin{aligned} &\left[i\hbar \frac{\partial}{\partial t} - \epsilon_j + \epsilon_i \right] \Delta_{ij}^{(1)}(t) \\ &= (n_i - n_j) \left[V_{ji}(t) + \sum_{kl} \Delta_{kl}^{(1)}(t) (U_{jkli} - U_{jkil}) \right], \end{aligned} \quad (4.73)$$

which is our desired result.

4.4.1 Bosonic representation of the low-energy excitations

We notice from (4.73) that the only expectation values which are influenced at linear order by the perturbation are those which either $n_i = 1$ and $n_j = 0$ or viceversa, namely where one of the index refer to an occupied state within (4.62) and the other to an un-occupied one. Let us denote by greek letters α, β, \dots the un-occupied states ($> N$), hereafter named “particles”, and by roman letters a, b, \dots the occupied ones ($\leq N$), named “holes”. We denote by

$$b_{\alpha a}^\dagger = c_\alpha^\dagger c_a, \quad (4.74)$$

the particle-hole creation operator, which destroys one electron (create one hole) inside the Slater determinant and creates it outside, and its hermitean conjugate

$$b_{\alpha a} = c_a^\dagger c_\alpha. \quad (4.75)$$

The commutators

$$[b_{\alpha a}, b_{\beta b}] = [b_{\alpha a}^\dagger, b_{\beta b}^\dagger] = 0,$$

vanish, while

$$[b_{\alpha a}, b_{\beta b}^\dagger] = \delta_{\alpha\beta} c_a^\dagger c_b - \delta_{ab} c_\beta^\dagger c_\alpha,$$

has the average value on (4.62) given by

$$\langle \Phi_{HF} | [b_{\alpha a}, b_{\beta b}^\dagger] | \Phi_{HF} \rangle = \delta_{\alpha\beta} \delta_{ab} (n_a - n_\alpha) = \delta_{\alpha\beta} \delta_{ab},$$

as if the particle-hole creation and annihilation operators were bosonic particles. If we assume that at linear order in V the Hartree-Fock wave-function is slightly modified with respect to its time-independent value, in other words we make a similar assumption as we did in deriving spin-wave theory, then we can approximate the commutator by its average value, thus obtaining

$$[b_{\alpha a}, b_{\beta b}^\dagger] = \delta_{\alpha\beta} \delta_{ab}, \quad [b_{\alpha a}, b_{\beta b}] = [b_{\alpha a}^\dagger, b_{\beta b}^\dagger] = 0, \quad (4.76)$$

which are indeed bosonic commutation relations. We notice that the bosonic vacuum is the time-independent Hartree-Fock wave-function. Since

$$\Delta_{aa}(t) = \langle \Phi_{HF}(t) | b_{\alpha a} | \Phi_{HF}(t) \rangle,$$

Eq. (4.73) implies the following equation of motion for the bosonic operators

$$\begin{aligned} & \left[i\hbar \frac{\partial}{\partial t} - \epsilon_\alpha + \epsilon_a \right] b_{\alpha a} \\ &= \left[V_{\alpha a}(t) + \sum_{\beta b} b_{\beta b} (U_{\alpha b \beta a} - U_{\alpha b a \beta}) + b_{\beta b}^\dagger (U_{\alpha \beta b a} - U_{\alpha \beta a b}) \right]. \end{aligned} \quad (4.77)$$

We may now ask the following question: What would be a bosonic Hamiltonian leading to the above equation of motion? The answer can be readily found and is

$$\begin{aligned} & \sum_{\alpha a} (\epsilon_\alpha - \epsilon_a) b_{\alpha a}^\dagger b_{\alpha a} + \sum_{\alpha \beta ab} b_{\alpha a}^\dagger b_{\beta b} (U_{\alpha b \beta a} - U_{\alpha b a \beta}) \\ &+ \frac{1}{2} \sum_{\alpha \beta ab} b_{\alpha a}^\dagger b_{\beta b}^\dagger (U_{\alpha \beta b a} - U_{\alpha \beta a b}) + b_{\beta b} b_{\alpha a} (U_{a b \beta \alpha} - U_{a b \alpha \beta}) \\ &+ \sum_{\alpha a} V_{\alpha a}(t) b_{\alpha a}^\dagger + V_{a \alpha}(t) b_{\alpha a}. \end{aligned} \quad (4.78)$$

It is now clear that the external field simply probes particle-hole excitations which have their own dynamics provided by the Hamiltonian

$$\begin{aligned} \hat{H}_{TDHF} &= \sum_{\alpha a} (\epsilon_\alpha - \epsilon_a) b_{\alpha a}^\dagger b_{\alpha a} + \sum_{\alpha \beta ab} b_{\alpha a}^\dagger b_{\beta b} (U_{\alpha b \beta a} - U_{\alpha b a \beta}) \\ &+ \frac{1}{2} \sum_{\alpha \beta ab} b_{\alpha a}^\dagger b_{\beta b}^\dagger (U_{\alpha \beta b a} - U_{\alpha \beta a b}) + b_{\beta b} b_{\alpha a} (U_{a b \beta \alpha} - U_{a b \alpha \beta}). \end{aligned} \quad (4.79)$$

Due to the presence of the last two terms, the true ground state of (4.79) is not the vacuum, namely the Hartree-Fock wave-function, but another state

$$|\Phi_{TDHF}\rangle = e^A |\Phi_{HF}\rangle,$$

with A an anti-hermitean operator quadratic in the bosonic operators. The above wave-function is actually an improvement of the Hartree-Fock wave-function that includes the zero-point fluctuations of the particle-hole excitations.

The above result can be re-derived in the spirit of the spin-wave theory, that we have already encountered, without even invoking the time-dependent Hartree-Fock. If we assume, to be checked *a posteriori*, that the Hartree-Fock wave-function is not strongly modified by the inclusion of quantum fluctuations, we can assume that the commutators

$$\begin{aligned} [c_a^\dagger c_\alpha, c_\beta^\dagger c_b] &= \delta_{\alpha\beta} c_a^\dagger c_b - \delta_{ab} c_\beta^\dagger c_\alpha, \\ [c_\alpha^\dagger c_a, c_b^\dagger c_\beta] &= \delta_{ab} c_\alpha^\dagger c_\beta - \delta_{\alpha\beta} c_b^\dagger c_a, \\ [c_a^\dagger c_b, c_c^\dagger c_d] &= \delta_{bc} c_a^\dagger c_d - \delta_{ad} c_c^\dagger c_b, \\ [c_\alpha^\dagger c_\beta, c_\gamma^\dagger c_\delta] &= \delta_{\beta\gamma} c_\alpha^\dagger c_\delta - \delta_{\alpha\delta} c_\gamma^\dagger c_\beta, \end{aligned}$$

can be effectively substituted by their average values on the Hartree-Fock wave-function, i.e.

$$\begin{aligned} [c_a^\dagger c_\alpha, c_\beta^\dagger c_b] &= \delta_{\alpha\beta} \delta_{ab}, \\ [c_\alpha^\dagger c_a, c_b^\dagger c_\beta] &= -\delta_{\alpha\beta} \delta_{ab}, \\ [c_a^\dagger c_b, c_c^\dagger c_d] &= 0, \\ [c_\alpha^\dagger c_\beta, c_\gamma^\dagger c_\delta] &= 0, \end{aligned}$$

which justifies the identification with bosonic operators. The only terms of the interaction that may have non vanishing effect when applied either on the right or on the left of the Hartree-Fock wave-functtion are those which contain two particle and two holes, hence they are

$$\begin{aligned} \mathcal{H}_{int} &\simeq \frac{1}{2} \sum_{ab\alpha\beta} U_{b\alpha\beta a} c_b^\dagger c_\alpha^\dagger c_\beta c_a + U_{\alpha b a \beta} c_\alpha^\dagger c_b^\dagger c_a c_\beta \\ &\quad + U_{b\alpha a \beta} c_b^\dagger c_\alpha^\dagger c_a c_\beta + U_{\alpha b \beta a} c_\alpha^\dagger c_b^\dagger c_\beta c_a \\ &\quad + U_{\alpha\beta b a} c_\alpha^\dagger c_\beta^\dagger c_b c_a + U_{a b \beta \alpha} c_a^\dagger c_b^\dagger c_\beta c_\alpha \\ &= \frac{1}{2} \sum_{ab\alpha\beta} 2(U_{\alpha b \beta a} - U_{\alpha b a \beta}) c_\alpha^\dagger c_b^\dagger c_\beta c_a \end{aligned}$$

$$+U_{\alpha\beta ba} c_\alpha^\dagger c_\beta^\dagger c_b c_a + U_{ab\beta\alpha} c_a^\dagger c_b^\dagger c_\beta c_\alpha.$$

Next we have to express the interaction in terms of bosons, avoiding double counting. The first term becomes straightforwardly

$$\sum_{ab\alpha\beta} \left(U_{ab\beta a} - U_{\alpha b a \beta} \right) b_{\alpha a}^\dagger b_{\beta b}.$$

The second term is more delicate to re-express, as one can at will couple α with a or b , thus getting either $b_{\alpha a}^\dagger b_{\beta b}^\dagger$ or $-b_{\alpha b}^\dagger b_{\beta a}^\dagger$. Although the two terms correspond to the same fermionic operator, they are independent from the bosonic point of view, hence they both have to be kept, leading to

$$\frac{1}{2} \sum_{ab\alpha\beta} \left(U_{\alpha\beta ba} - U_{\alpha\beta ab} \right) b_{\alpha a}^\dagger b_{\beta b}^\dagger + H.c.,$$

which coincides with the term in (4.79).

4.5 Application: antiferromagnetism in the half-filled Hubbard model

Let us consider again the Hubbard model on an hypercubic lattice in d -dimensions:

$$\mathcal{H} = -t \sum_{\langle \mathbf{R}\mathbf{R}' \rangle} \sum_{\sigma} \left(c_{\mathbf{R}\sigma}^{\dagger} c_{\mathbf{R}'\sigma} + H.c. \right) + U \sum_{\mathbf{R}} \hat{n}_{\mathbf{R}\uparrow} \hat{n}_{\mathbf{R}\downarrow}, \quad (4.80)$$

where

$$\hat{n}_{\mathbf{R}\sigma} = c_{\mathbf{R}\sigma}^{\dagger} c_{\mathbf{R}\sigma},$$

and, as usual, $\langle \mathbf{R}\mathbf{R}' \rangle$ means that \mathbf{R} and \mathbf{R}' are nearest neighbor sites. We already showed that for very large U/t and one electron per site, i.e. half-filling, this model is a Mott insulator with a Ne l magnetic order in $d > 1$ at zero temperature and in $d > 2$ at finite temperature below a critical T_c . Let us now try to recover this behavior within the previously described Hartree-Fock theory.

The first step is to identify the variational parameters. The interaction, being on-site, leads to local variational parameters which are

$$\Delta_{\mathbf{R},\sigma\sigma'} = \langle \Phi_{HF} | c_{\mathbf{R}\sigma}^{\dagger} c_{\mathbf{R}\sigma'} | \Phi_{HF} \rangle.$$

We search for an Hartree-Fock Slater determinant which describes a Ne l order with the antiferromagnetic order parameter along the z -direction, namely we assume that the spin SU(2) symmetry is lowered down to a U(1) symmetry which describes spin-rotations around the z -axis. This implies that we can choose $|\Phi_{HF}\rangle$ as an eigenstate of the z -component of the total spin, hence that the only finite variational parameters are diagonal in the spin index, namely

$$n_{\mathbf{R}\sigma} = \langle \Phi_{HF} | \hat{n}_{\mathbf{R}\sigma} | \Phi_{HF} \rangle.$$

Since the average number of electrons per site is $\sum_{\sigma} n_{\mathbf{R}\sigma} = 1$, we use the following parametrization:

$$n_{\mathbf{R}\uparrow} = \frac{1}{2} + m (-1)^R, \quad (4.81)$$

$$n_{\mathbf{R}\downarrow} = \frac{1}{2} - m (-1)^R, \quad (4.82)$$

where if the vector $\mathbf{R} = a(n_1, n_2, \dots, n_d)$, a being the lattice spacing, then $R = \sum_{i=1}^d n_i$. In other words the average magnetization is assumed to be

$$S_{\mathbf{R}}^z = \frac{1}{2} (n_{\mathbf{R}\uparrow} - n_{\mathbf{R}\downarrow}) = m (-1)^R.$$

The Hartree-Fock Hamiltonian is therefore

$$\begin{aligned}\mathcal{H}_{HF} &= -t \sum_{\langle \mathbf{R} \mathbf{R}' \rangle} \sum_{\sigma} c_{\mathbf{R} \sigma}^{\dagger} c_{\mathbf{R}' \sigma} + H.c. + U \sum_{\mathbf{R}} (\hat{n}_{\mathbf{R} \uparrow} n_{\mathbf{R} \downarrow} + \hat{n}_{\mathbf{R} \downarrow} n_{\mathbf{R} \uparrow}) \\ &= -t \sum_{\langle \mathbf{R} \mathbf{R}' \rangle} \sum_{\sigma} c_{\mathbf{R} \sigma}^{\dagger} c_{\mathbf{R}' \sigma} + H.c. - U m \sum_{\mathbf{R}} (-1)^R (\hat{n}_{\mathbf{R} \uparrow} - \hat{n}_{\mathbf{R} \downarrow}) \\ &\quad + \frac{U}{2} \sum_{\mathbf{R}} (\hat{n}_{\mathbf{R} \uparrow} + \hat{n}_{\mathbf{R} \downarrow}).\end{aligned}$$

The last term is proportional to the total number of electrons, $UN/2$, which is a conserved quantity. Therefore $UN/2$ is just a constant which can be dropped leading to the Hartree-Fock Hamiltonian

$$\mathcal{H}_{HF} = -t \sum_{\langle \mathbf{R} \mathbf{R}' \rangle} \sum_{\sigma} c_{\mathbf{R} \sigma}^{\dagger} c_{\mathbf{R}' \sigma} + H.c. - U m \sum_{\mathbf{R}} (-1)^R (\hat{n}_{\mathbf{R} \uparrow} - \hat{n}_{\mathbf{R} \downarrow}). \quad (4.83)$$

Let us write this Hamiltonian in momentum space. Since

$$(-1)^R = e^{i\mathbf{Q} \cdot \mathbf{R}},$$

where $\mathbf{Q} = \pi(1, 1, \dots, 1)/a$, one readily finds that

$$\mathcal{H}_{HF} = \sum_{\mathbf{k} \sigma} \epsilon_{\mathbf{k}} \hat{n}_{\mathbf{k} \sigma} - U m \sum_{\mathbf{k}} \left(c_{\mathbf{k} \uparrow}^{\dagger} c_{\mathbf{k} + \mathbf{Q} \uparrow} - c_{\mathbf{k} \downarrow}^{\dagger} c_{\mathbf{k} + \mathbf{Q} \downarrow} \right). \quad (4.84)$$

If $\mathbf{k} = (k_1, k_2, \dots, k_d)$, the bare dispersion is given by

$$\epsilon_{\mathbf{k}} = -2t \sum_{i=1}^d \cos k_i a.$$

The original Brillouin zone is an hypercube with linear size $2\pi/a$. Since the Hartree-Fock Hamiltonian breaks translational symmetry – the new unit cell is twice larger – the actual Brillouin zone is half the original one. Let us define the new Brillouin zone, which we call *Magnetic Brillouin zone* (MBZ) as the volume which encloses all \mathbf{k} -points such that $\epsilon_{\mathbf{k}} \leq 0$. Since for any of these points

$$\epsilon_{\mathbf{k} + \mathbf{Q}} = -\epsilon_{\mathbf{k}} \geq 0,$$

the MBZ is indeed twice-smaller than the original one. Then let us define new fermionic operators with $\mathbf{k} \in MBZ$ by

$$a_{\mathbf{k} \sigma} = c_{\mathbf{k} \sigma}, \quad b_{\mathbf{k} \sigma} = c_{\mathbf{k} + \mathbf{Q} \sigma},$$

and spinorial operators

$$\psi_{\mathbf{k} \sigma} = \begin{pmatrix} a_{\mathbf{k} \sigma} \\ b_{\mathbf{k} \sigma} \end{pmatrix}. \quad (4.85)$$

In terms of the latter (4.84) can be written as

$$\mathcal{H}_{HF} = \sum_{\mathbf{k} \in MBZ \sigma} \epsilon_{\mathbf{k}} \psi_{\mathbf{k}\sigma}^\dagger \tau_3 \psi_{\mathbf{k}\sigma} - U m \sum_{\mathbf{k} \in MBZ} \psi_{\mathbf{k}\uparrow}^\dagger \tau_1 \psi_{\mathbf{k}\uparrow} - \psi_{\mathbf{k}\downarrow}^\dagger \tau_1 \psi_{\mathbf{k}\downarrow}, \quad (4.86)$$

where τ_i 's, $i = 1, 2, 3$, are Pauli matrices acting in the spinorial basis. We notice that

$$\begin{aligned} \epsilon_{\mathbf{k}} \tau_3 \mp U m \tau_1 &= -E_{\mathbf{k}} \tau_3 \left(-\frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}} \pm i \frac{Um}{E_{\mathbf{k}}} \tau_2 \right) \\ &= -E_{\mathbf{k}} \tau_3 e^{\pm 2i\theta_{\mathbf{k}} \tau_2} = -E_{\mathbf{k}} e^{\mp i\theta_{\mathbf{k}} \tau_2} \tau_3 e^{\pm i\theta_{\mathbf{k}} \tau_2}, \end{aligned}$$

where

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + U^2 m^2}, \quad (4.87)$$

and

$$\cos 2\theta_{\mathbf{k}} = -\frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}, \quad \sin 2\theta_{\mathbf{k}} = \frac{Um}{E_{\mathbf{k}}}.$$

Therefore if we define two new spinors through

$$\phi_{\mathbf{k}\uparrow} = \begin{pmatrix} \alpha_{\mathbf{k}\uparrow} \\ \beta_{\mathbf{k}\uparrow} \end{pmatrix} = e^{i\theta_{\mathbf{k}} \tau_2} \psi_{\mathbf{k}\uparrow}, \quad \phi_{\mathbf{k}\downarrow} = \begin{pmatrix} \alpha_{\mathbf{k}\downarrow} \\ \beta_{\mathbf{k}\downarrow} \end{pmatrix} = e^{-i\theta_{\mathbf{k}} \tau_2} \psi_{\mathbf{k}\downarrow}, \quad (4.88)$$

the Hamiltonian becomes

$$\mathcal{H}_{HF} = - \sum_{\mathbf{k} \in MBZ \sigma} E_{\mathbf{k}} \phi_{\mathbf{k}\sigma}^\dagger \tau_3 \phi_{\mathbf{k}\sigma} = - \sum_{\mathbf{k} \in MBZ \sigma} E_{\mathbf{k}} (\alpha_{\mathbf{k}\sigma}^\dagger \alpha_{\mathbf{k}\sigma} - \beta_{\mathbf{k}\sigma}^\dagger \beta_{\mathbf{k}\sigma}), \quad (4.89)$$

namely it acquires a diagonal form. Since $E_{\mathbf{k}} > 0$ the ground state with a number of electrons equal to the number of sites N is simply obtained by filling completely the α -band (notice that the MBZ contains $N/2$ \mathbf{k} -points, hence each band can accommodate $2N/2 = N$ electrons). Thus the Hartree-Fock Hamiltonian describes a band-insulator with two bands separated by a gap of minimal value $2U m$. The Hartree-Fock wave-function satisfies:

$$\langle \Phi_{HF} | \phi_{\mathbf{k}\sigma}^\dagger \tau_i \phi_{\mathbf{k}\sigma} | \Phi_{HF} \rangle = \delta_{i3},$$

which becomes at finite temperature

$$\langle \phi_{\mathbf{k}\sigma}^\dagger \tau_i \phi_{\mathbf{k}\sigma} \rangle = \delta_{i3} \tanh \frac{E_{\mathbf{k}}}{2T}. \quad (4.90)$$

We still have to impose the self-consistency condition

$$m = \frac{1}{2V} \sum_{\mathbf{R}} (-1)^R \langle \hat{n}_{\mathbf{R}\uparrow} - \hat{n}_{\mathbf{R}\downarrow} \rangle$$

$$\begin{aligned}
&= \frac{1}{2V} \sum_{\mathbf{k} \in MBZ} \langle \psi_{\mathbf{k}\uparrow}^\dagger \tau_1 \psi_{\mathbf{k}\uparrow} - \psi_{\mathbf{k}\downarrow}^\dagger \tau_1 \psi_{\mathbf{k}\downarrow} \rangle \\
&= \frac{1}{2V} \sum_{\mathbf{k} \in MBZ} \langle \psi_{\mathbf{k}\uparrow}^\dagger e^{i\theta_{\mathbf{k}} \tau_2} \tau_1 e^{-i\theta_{\mathbf{k}} \tau_2} \psi_{\mathbf{k}\uparrow} - \psi_{\mathbf{k}\downarrow}^\dagger e^{-i\theta_{\mathbf{k}} \tau_2} \tau_1 e^{i\theta_{\mathbf{k}} \tau_2} \psi_{\mathbf{k}\downarrow} \rangle \\
&= \frac{1}{2V} \sum_{\mathbf{k} \in MBZ} \langle \phi_{\mathbf{k}\uparrow}^\dagger (\cos 2\theta_{\mathbf{k}} \tau_1 + \sin 2\theta_{\mathbf{k}} \tau_3) \phi_{\mathbf{k}\uparrow} - \phi_{\mathbf{k}\downarrow}^\dagger (\cos 2\theta_{\mathbf{k}} \tau_1 - \sin 2\theta_{\mathbf{k}} \tau_3) \phi_{\mathbf{k}\downarrow} \rangle \\
&= \frac{1}{V} \sum_{\mathbf{k} \in MBZ} \sin 2\theta_{\mathbf{k}} \tanh \frac{E_{\mathbf{k}}}{2T}.
\end{aligned}$$

In other words the self-consistency condition reads

$$\frac{U}{2V} \sum_{\mathbf{k}} \frac{1}{E_{\mathbf{k}}} \tanh \frac{E_{\mathbf{k}}}{2T} = 1. \quad (4.91)$$

We solve this self-consistency condition by assuming a constant density of states, namely

$$\frac{1}{V} \sum_{\mathbf{k}} \dots = \int d\epsilon \rho(\epsilon) \dots \rightarrow \rho_0 \int_{-D}^D d\epsilon \dots,$$

where $\rho_0 = 1/2D$, with $D \sim 2dt$. At zero temperature we find

$$1 = \frac{U\rho_0}{2} \int_{-D}^D d\epsilon \frac{1}{\sqrt{\epsilon^2 + U^2 m^2}},$$

which has solution given by

$$m = \frac{D}{U} \left(\sinh \frac{1}{U\rho_0} \right)^{-1}.$$

This equation has always a solution for any $U \neq 0$. In particular, for $U \ll D$,

$$m \simeq \frac{D}{U} \exp \left(-\frac{1}{U\rho_0} \right). \quad (4.92)$$

This results states that the Hubbard model at half-filling on an hypercubic lattice is always an antiferromagnetic insulator whatever is the value of the Hubbard U . Notice that in the opposite limit of $U \gg D$, $m \sim D\rho_0 = 1/2$, which is the expected result since, for large U , electrons localize, one per site, hence behave like local spin-1/2 moments.

We can also determine the Néel temperature, which is the temperature T_c at which the self-consistency condition starts to be verified with $m = 0$, namely

$$1 = \frac{U}{2V} \sum_{\mathbf{k}} \frac{1}{\epsilon_{\mathbf{k}}} \tanh \frac{\epsilon_{\mathbf{k}}}{2T_c} \simeq \frac{U\rho_0}{2} \int_{-D}^D \frac{d\epsilon}{\epsilon} \tanh \frac{\epsilon}{2T_c}. \quad (4.93)$$

One finds that $T_c \sim U m(T = 0)$. This implies that

$$T_c \sim D \exp\left(-\frac{1}{U\rho_0}\right),$$

for small U , but $T_c \sim U$ at large U . The latter results contradicts what we previously found in the large U limit, by mapping the Hubbard model onto an Heisenberg model. There, within spin-wave theory, we showed that $T_c \sim J \sim t^2/U$, hence vanishes for large U . The origin of the disagreement stems from the fact that the Hartree-Fock theory is valid only for an interaction which is weak compared to the electron bandwidth. Essentially the Mott phenomenon, which dominates at large U/t , escapes any description using a single Slater determinant, which is only able to mimick a band-insulator.

4.5.1 Spin-wave spectrum by time dependent Hartree-Fock

Rigorously speaking, Hartree-Fock theory only allows to access ground state or, at finite temperature, equilibrium properties, although in an approximate variational manner, but not properties of excited states. Therefore it is not legitimate to interpret the spectrum of the Hartree-Fock Hamiltonian as an approximation of the actual spectrum. For instance we showed that the Heisenberg antiferromagnet, which corresponds to the large U -limit of the Hubbard model at half-filling, has gapless spin-wave excitations. On the contrary the Hartree-Fock Hamiltonian, which describes a band-insulator, has a gap for all excitations. The simplest way to cure this defect, namely to have access to excitations, is by means of the time dependent Hartree-Fock. Here we apply this technique to recover the spin-wave spectrum.

Let us derive the bosonic Hamiltonian for the spin-flip particle-hole excitations above the Hartree-Fock ground state. We consider, in terms of the spinors (4.88) which diagonalize the Hartree-Fock Hamiltonian, the following spin-flip operators:

$$\begin{aligned} X_{\mathbf{k};\mathbf{q}} &= \sqrt{\frac{1}{2}} \phi_{\mathbf{k}\uparrow}^\dagger \tau_1 \phi_{\mathbf{k}+\mathbf{q}\downarrow}, \\ X_{\mathbf{k};\mathbf{q}}^\dagger &= \sqrt{\frac{1}{2}} \phi_{\mathbf{k}+\mathbf{q}\downarrow}^\dagger \tau_1 \phi_{\mathbf{k}\uparrow}, \\ P_{\mathbf{k};\mathbf{q}} &= \sqrt{\frac{1}{2}} \phi_{\mathbf{k}\uparrow}^\dagger \tau_2 \phi_{\mathbf{k}+\mathbf{q}\downarrow}, \\ P_{\mathbf{k};\mathbf{q}}^\dagger &= \sqrt{\frac{1}{2}} \phi_{\mathbf{k}+\mathbf{q}\downarrow}^\dagger \tau_2 \phi_{\mathbf{k}\uparrow}. \end{aligned}$$

In the framework of time-dependent Hartree-Fock one can assume that

$$\left[X_{\mathbf{k};\mathbf{q}}, P_{\mathbf{k}';\mathbf{q}'}^\dagger \right] = \frac{i}{2} \left(\delta_{\mathbf{k}+\mathbf{q},\mathbf{k}'+\mathbf{q}'} \phi_{\mathbf{k}\uparrow}^\dagger \tau_3 \phi_{\mathbf{k}'\uparrow} + \delta_{\mathbf{k},\mathbf{k}'} \phi_{\mathbf{k}'+\mathbf{q}'\downarrow}^\dagger \tau_3 \phi_{\mathbf{k}+\mathbf{q}\downarrow} \right)$$

$$\simeq \langle \Phi_{HF} | \left[X_{\mathbf{k};\mathbf{q}}, P_{\mathbf{k}';\mathbf{q}'}^\dagger \right] | \Phi_{HF} \rangle = i \delta_{\mathbf{k},\mathbf{k}'} \delta_{\mathbf{q},\mathbf{q}'},$$

which shows that X and P^\dagger are conjugate variables. The energy cost of such spin-flip excitations are described by the free Hamiltonian

$$\mathcal{H}_0 = \sum_{\mathbf{k} \mathbf{q}} \omega_{\mathbf{k};\mathbf{q}} \left(X_{\mathbf{k};\mathbf{q}}^\dagger X_{\mathbf{k};\mathbf{q}} + P_{\mathbf{k};\mathbf{q}}^\dagger P_{\mathbf{k};\mathbf{q}} \right), \quad (4.94)$$

where

$$\omega_{\mathbf{k};\mathbf{q}} = E_{\mathbf{k}+\mathbf{q}} + E_{\mathbf{k}}.$$

This simply means that if one destroys an α particle at \mathbf{k} and create a β one at $\mathbf{k}+\mathbf{q}$, the energy cost is $\omega_{\mathbf{k};\mathbf{q}}$.

Following the prescriptions of time-dependent Hartree-Fock, we still need to express the Hubbard interaction in terms of these spin-flip excitations. We notice that

$$\begin{aligned} \hat{n}_{\mathbf{R}\uparrow} \hat{n}_{\mathbf{R}\downarrow} &= c_{\mathbf{R}\uparrow}^\dagger c_{\mathbf{R}\uparrow} c_{\mathbf{R}\downarrow}^\dagger c_{\mathbf{R}\downarrow} \\ &= -c_{\mathbf{R}\uparrow}^\dagger c_{\mathbf{R}\downarrow} c_{\mathbf{R}\downarrow}^\dagger c_{\mathbf{R}\uparrow} \equiv S_{\mathbf{R}}^+ S_{\mathbf{R}}^-, \end{aligned}$$

so that

$$U \sum_{\mathbf{R}} \hat{n}_{\mathbf{R}\uparrow} \hat{n}_{\mathbf{R}\downarrow} = U \sum_{\mathbf{R}} S_{\mathbf{R}}^+ S_{\mathbf{R}}^- = \frac{U}{V} \sum_{\mathbf{q}} S_{\mathbf{q}}^+ S_{-\mathbf{q}}^-,$$

where

$$S_{\mathbf{q}}^+ = \sum_{\mathbf{R}} e^{-i\mathbf{q}\cdot\mathbf{R}} S_{\mathbf{R}}^+ = \sum_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}+\mathbf{q}\downarrow}.$$

We recall that the MBZ is half the original one. For instance, while before the momenta $\mathbf{q} = \mathbf{0}$ and $\mathbf{q} = \mathbf{Q}$ were different, in the MBZ both coincide with momentum zero. Therefore, if we are interested in long wavelength excitations, we need to consider in the original BZ both $\mathbf{q} \sim \mathbf{0}$ and $\mathbf{q} \sim \mathbf{Q}$. For $\mathbf{q} \sim \mathbf{0}$, $S_{\mathbf{q}}^+$ connects states inside the MBZ, i.e.

$$S_{\mathbf{q}}^+ \simeq \sum_{\mathbf{k} \in MBZ} a_{\mathbf{k}\uparrow}^\dagger a_{\mathbf{k}+\mathbf{q}\downarrow} + b_{\mathbf{k}\uparrow}^\dagger b_{\mathbf{k}+\mathbf{q}\downarrow} = \sum_{\mathbf{k} \in MBZ} \psi_{\mathbf{k}\uparrow}^\dagger \psi_{\mathbf{k}+\mathbf{q}\downarrow}.$$

Near \mathbf{Q} we can consider the operator $S_{\mathbf{q}+\mathbf{Q}}^+$ with small \mathbf{q} , which is

$$S_{\mathbf{q}+\mathbf{Q}}^+ \simeq \sum_{\mathbf{k} \in MBZ} a_{\mathbf{k}\uparrow}^\dagger b_{\mathbf{k}+\mathbf{q}\downarrow} + b_{\mathbf{k}\uparrow}^\dagger a_{\mathbf{k}+\mathbf{q}\downarrow} = \sum_{\mathbf{k} \in MBZ} \psi_{\mathbf{k}\uparrow}^\dagger \tau_1 \psi_{\mathbf{k}+\mathbf{q}\downarrow}.$$

Therefore in the long wavelength limit it is legitimate to re-write

$$\frac{U}{V} \sum_{\mathbf{q}} S_{\mathbf{q}}^+ S_{-\mathbf{q}}^- = \frac{U}{V} \sum_{\mathbf{k} \mathbf{p} \mathbf{q} \in MBZ} \psi_{\mathbf{k}\uparrow}^\dagger \psi_{\mathbf{k}+\mathbf{q}\downarrow} \psi_{\mathbf{p}+\mathbf{q}\downarrow}^\dagger \psi_{\mathbf{p}\uparrow} + \psi_{\mathbf{k}\uparrow}^\dagger \tau_1 \psi_{\mathbf{k}+\mathbf{q}\downarrow} \psi_{\mathbf{p}+\mathbf{q}\downarrow}^\dagger \tau_1 \psi_{\mathbf{p}\uparrow}.$$

Notice that

$$\begin{aligned}\psi_{\mathbf{k}\uparrow}^\dagger \psi_{\mathbf{k}+\mathbf{q}\downarrow} &= \phi_{\mathbf{k}\uparrow}^\dagger e^{i\theta_{\mathbf{k}}\tau_2} e^{i\theta_{\mathbf{k}+\mathbf{q}}\tau_2} \phi_{\mathbf{k}+\mathbf{q}\downarrow} \\ &\simeq i \sin(\theta_{\mathbf{k}} + \theta_{\mathbf{k}+\mathbf{q}}) \phi_{\mathbf{k}\uparrow}^\dagger \tau_2 \phi_{\mathbf{k}+\mathbf{q}\downarrow} = i\sqrt{2} \sin(\theta_{\mathbf{k}} + \theta_{\mathbf{k}+\mathbf{q}}) P_{\mathbf{k};\mathbf{q}}, \\ \psi_{\mathbf{k}\uparrow}^\dagger \tau_1 \psi_{\mathbf{k}+\mathbf{q}\downarrow} &= \phi_{\mathbf{k}\uparrow}^\dagger e^{i\theta_{\mathbf{k}}\tau_2} \tau_1 e^{i\theta_{\mathbf{k}+\mathbf{q}}\tau_2} \phi_{\mathbf{k}+\mathbf{q}\downarrow} \\ &\simeq \cos(\theta_{\mathbf{k}} - \theta_{\mathbf{k}+\mathbf{q}}) \phi_{\mathbf{k}\uparrow}^\dagger \tau_1 \phi_{\mathbf{k}+\mathbf{q}\downarrow} = \sqrt{2} \cos(\theta_{\mathbf{k}} - \theta_{\mathbf{k}+\mathbf{q}}) X_{\mathbf{k};\mathbf{q}},\end{aligned}$$

so that the interaction Hamiltonian becomes

$$\begin{aligned}\mathcal{H}_{int} &= -\frac{2U}{V} \sum_{\mathbf{k} \mathbf{p} \mathbf{q} \in MBZ} \sin(\theta_{\mathbf{k}} + \theta_{\mathbf{k}+\mathbf{q}}) \sin(\theta_{\mathbf{p}} + \theta_{\mathbf{p}+\mathbf{q}}) P_{\mathbf{k};\mathbf{q}}^\dagger P_{\mathbf{p};\mathbf{q}} \\ &\quad + \cos(\theta_{\mathbf{k}} - \theta_{\mathbf{k}+\mathbf{q}}) \cos(\theta_{\mathbf{p}} - \theta_{\mathbf{p}+\mathbf{q}}) X_{\mathbf{k};\mathbf{q}}^\dagger X_{\mathbf{p};\mathbf{q}}.\end{aligned}\tag{4.95}$$

The complete Hamiltonian for the spin-flip excitations is therefore

$$\begin{aligned}\mathcal{H} &= \sum_{\mathbf{k} \mathbf{q} \in MBZ} \omega_{\mathbf{k};\mathbf{q}} \left(X_{\mathbf{k};\mathbf{q}}^\dagger X_{\mathbf{k};\mathbf{q}} + P_{\mathbf{k};\mathbf{q}}^\dagger P_{\mathbf{k};\mathbf{q}} \right) \\ &\quad - \frac{2U}{V} \sum_{\mathbf{k} \mathbf{p} \mathbf{q} \in MBZ} \sin(\theta_{\mathbf{k}} + \theta_{\mathbf{k}+\mathbf{q}}) \sin(\theta_{\mathbf{p}} + \theta_{\mathbf{p}+\mathbf{q}}) P_{\mathbf{k};\mathbf{q}}^\dagger P_{\mathbf{p};\mathbf{q}} \\ &\quad + \cos(\theta_{\mathbf{k}} - \theta_{\mathbf{k}+\mathbf{q}}) \cos(\theta_{\mathbf{p}} - \theta_{\mathbf{p}+\mathbf{q}}) X_{\mathbf{k};\mathbf{q}}^\dagger X_{\mathbf{p};\mathbf{q}}.\end{aligned}\tag{4.96}$$

One might diagonalize this Hamiltonian to obtain the spin-flip excitation spectrum. Here we aim simply to show that (4.96) does contain the spin-waves.

First we perform the canonical transformation

$$\begin{aligned}X_{\mathbf{k};\mathbf{q}} &\rightarrow \sqrt{\frac{1}{\omega_{\mathbf{k};\mathbf{q}}}} X_{\mathbf{k};\mathbf{q}}, \\ P_{\mathbf{k};\mathbf{q}} &\rightarrow \sqrt{\omega_{\mathbf{k};\mathbf{q}}} P_{\mathbf{k};\mathbf{q}},\end{aligned}$$

after which

$$\begin{aligned}\mathcal{H} &= \sum_{\mathbf{k} \mathbf{q} \in MBZ} X_{\mathbf{k};\mathbf{q}}^\dagger X_{\mathbf{k};\mathbf{q}} + \omega_{\mathbf{k};\mathbf{q}}^2 P_{\mathbf{k};\mathbf{q}}^\dagger P_{\mathbf{k};\mathbf{q}} \\ &\quad - \frac{2U}{V} \sum_{\mathbf{k} \mathbf{p} \mathbf{q} \in MBZ} \sqrt{\omega_{\mathbf{k};\mathbf{q}} \omega_{\mathbf{p};\mathbf{q}}} \sin(\theta_{\mathbf{k}} + \theta_{\mathbf{k}+\mathbf{q}}) \sin(\theta_{\mathbf{p}} + \theta_{\mathbf{p}+\mathbf{q}}) P_{\mathbf{k};\mathbf{q}}^\dagger P_{\mathbf{p};\mathbf{q}} \\ &\quad + \sqrt{\frac{1}{\omega_{\mathbf{k};\mathbf{q}} \omega_{\mathbf{p};\mathbf{q}}}} \cos(\theta_{\mathbf{k}} - \theta_{\mathbf{k}+\mathbf{q}}) \cos(\theta_{\mathbf{p}} - \theta_{\mathbf{p}+\mathbf{q}}) X_{\mathbf{k};\mathbf{q}}^\dagger X_{\mathbf{p};\mathbf{q}}.\end{aligned}$$

Next we make a unitary transformation and define the new operators

$$\begin{aligned}\tilde{X}_{\mathbf{q}} &= \sqrt{\frac{1}{\sum_{\mathbf{k} \in MBZ} \cos^2(\theta_{\mathbf{k}} - \theta_{\mathbf{k}+\mathbf{q}}) / \omega_{\mathbf{k};\mathbf{q}}}} \sum_{\mathbf{p} \in MBZ} \frac{\cos(\theta_{\mathbf{p}} - \theta_{\mathbf{p}+\mathbf{q}})}{\sqrt{\omega_{\mathbf{p};\mathbf{q}}}} X_{\mathbf{p};\mathbf{q}}, \\ \tilde{P}_{\mathbf{q}} &= \sqrt{\frac{1}{\sum_{\mathbf{k} \in MBZ} \cos^2(\theta_{\mathbf{k}} - \theta_{\mathbf{k}+\mathbf{q}}) / \omega_{\mathbf{k};\mathbf{q}}}} \sum_{\mathbf{p} \in MBZ} \frac{\cos(\theta_{\mathbf{p}} - \theta_{\mathbf{p}+\mathbf{q}})}{\sqrt{\omega_{\mathbf{p};\mathbf{q}}}} P_{\mathbf{p};\mathbf{q}},\end{aligned}$$

as well as all the other orthogonal combinations, $X_{i;\mathbf{q}}$ and $P_{i;\mathbf{q}}$. The part of the Hamiltonian which involves \tilde{X} is simply

$$\sum_{\mathbf{q} \in MBZ} \left(1 - \frac{2U}{V} \sum_{\mathbf{k} \in MBZ} \frac{\cos^2(\theta_{\mathbf{k}} - \theta_{\mathbf{k}+\mathbf{q}})}{\omega_{\mathbf{k};\mathbf{q}}} \right) \tilde{X}_{\mathbf{q}}^\dagger \tilde{X}_{\mathbf{q}}.$$

Notice that for $\mathbf{q} = 0$ the square bracket vanishes because is nothing but the self-consistency equation (4.91) at zero temperature, namely

$$1 = \frac{U}{V} \sum_{\mathbf{k} \in MBZ} \frac{1}{E_{\mathbf{k}}}.$$

Therefore for small \mathbf{q}

$$1 - \frac{2U}{V} \sum_{\mathbf{k} \in MBZ} \frac{\cos^2(\theta_{\mathbf{k}} - \theta_{\mathbf{k}+\mathbf{q}})}{\omega_{\mathbf{k};\mathbf{q}}} \sim A |\mathbf{q}|^2,$$

where A is a constant which can be determined and for large U/t behaves as t^2/U^2 . All the combinations of X 's, $X_{i;\mathbf{q}}$'s, which are orthogonal to \tilde{X} remain degenerate and described by the term

$$\sum_i \sum_{\mathbf{q}} X_{i;\mathbf{q}}^\dagger X_{i;\mathbf{q}}.$$

One realizes that the above $|\mathbf{q}|^2$ -term is the leading one at small \mathbf{q} , hence we can evaluate what is left putting $\mathbf{q} = 0$. Then, through (4.91), we find that

$$\tilde{P}_{\mathbf{q}} \simeq \sqrt{\frac{U}{V}} \sum_{\mathbf{k} \in MBZ} \sqrt{\frac{1}{E_{\mathbf{k}}}} P_{\mathbf{k};\mathbf{q}},$$

and that the part of the Hamiltonian involving the conjugate variables is

$$\sum_{\mathbf{k} \mathbf{q} \in MBZ} 4E_{\mathbf{k}}^2 P_{\mathbf{k};\mathbf{q}}^\dagger P_{\mathbf{k};\mathbf{q}} - \frac{2U}{V} \sum_{\mathbf{k} \mathbf{p} \mathbf{q} \in MBZ} 2\sqrt{E_{\mathbf{k}} E_{\mathbf{p}}} \frac{Um}{E_{\mathbf{k}}} \frac{Um}{E_{\mathbf{p}}} P_{\mathbf{k};\mathbf{q}}^\dagger P_{\mathbf{p};\mathbf{q}}$$

$$= \sum_{\mathbf{k}, \mathbf{q} \in MBZ} 4E_{\mathbf{k}}^2 P_{\mathbf{k};\mathbf{q}}^\dagger P_{\mathbf{k};\mathbf{q}} - 4U^2 m^2 \sum_{\mathbf{q}} \tilde{P}_{\mathbf{q}}^\dagger \tilde{P}_{\mathbf{q}}.$$

This implies that the conjugate variables are governed, at small \mathbf{q} , by the term

$$\sum_{\mathbf{q}} \left[\frac{4U}{V} \sum_{\mathbf{k} \in MBZ} E_{\mathbf{k}} - 4U^2 m^2 \right] \tilde{P}_{\mathbf{q}}^\dagger \tilde{P}_{\mathbf{q}} = B \sum_{\mathbf{q}} \tilde{P}_{\mathbf{q}}^\dagger \tilde{P}_{\mathbf{q}},$$

where $B \sim t^2$ for large U , and a bunch of other terms involving the orthogonal combinations $P_{i;\mathbf{q}}$'s which are coupled together and to $\tilde{P}_{\mathbf{q}}$. Let us neglect for the moment the coupling to $\tilde{P}_{\mathbf{q}}$. Then $\tilde{X}_{\mathbf{q}}$ and $\tilde{P}_{\mathbf{q}}$ are governed by the Hamiltonian

$$\sum_{\mathbf{q}} A|\mathbf{q}|^2 \tilde{X}_{\mathbf{q}}^\dagger \tilde{X}_{\mathbf{q}} + B \tilde{P}_{\mathbf{q}}^\dagger \tilde{P}_{\mathbf{q}},$$

which is diagonalized by the transformation $\tilde{X}_{\mathbf{q}} \rightarrow \sqrt{K_{\mathbf{q}}} \tilde{X}_{\mathbf{q}}$ and $\tilde{P}_{\mathbf{q}} \rightarrow \sqrt{K_{\mathbf{q}}^{-1}} \tilde{P}_{\mathbf{q}}$, where

$$K_{\mathbf{q}}^2 = \frac{B}{A|\mathbf{q}|^2},$$

leading to a linear dispersion

$$\omega_{\mathbf{q}} = \sqrt{AB} |\mathbf{q}| \sim J |\mathbf{q}|.$$

If we diagonalize the Hamiltonian which involves all other orthogonal combinations, we would get for them a gaped spectrum.

Notice that

$$\tilde{P}_{\mathbf{q}} \rightarrow \sqrt{K_{\mathbf{q}}^{-1}} \tilde{P}_{\mathbf{q}} \sim \sqrt{|\mathbf{q}|} \tilde{P}_{\mathbf{q}},$$

therefore the coupling between \tilde{P} and all other P_i 's is proportional to $\sqrt{|\mathbf{q}|}$ hence just renormalizes the spin-wave velocity. Moreover this coupling term between \tilde{P} and all P_i 's actually vanishes for large U since

$$\sum_{\mathbf{k}, \mathbf{q} \in MBZ} 4E_{\mathbf{k}}^2 P_{\mathbf{k};\mathbf{q}}^\dagger P_{\mathbf{k};\mathbf{q}} \sim 4U^2 m^2 \sum_{\mathbf{q}} \left[\tilde{P}_{\mathbf{q}}^\dagger \tilde{P}_{\mathbf{q}} + \sum_i P_{i;\mathbf{q}}^\dagger P_{i;\mathbf{q}} \right].$$

so that, for $U/t \gg 1$, the spin-wave velocity v is, up to subleading terms,

$$v = \sqrt{AB}, \quad (4.97)$$

with A and B defined previously.

4.6 Linear response of an electron gas

Let us consider now the response to an electromagnetic field of a solid. We start from the classical macroscopic Maxwell equations of an isolated system

$$\left\{ \begin{array}{lcl} \nabla \cdot \mathbf{E} & = & 4\pi\rho, \\ \nabla \cdot \mathbf{B} & = & 0, \\ \nabla \wedge \mathbf{E} & = & -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t}, \\ \nabla \wedge \mathbf{B} & = & \frac{1}{c}\frac{\partial \mathbf{E}}{\partial t} + \frac{4\pi}{c}\mathbf{J}, \end{array} \right. \quad (4.98)$$

where ρ is the total charge density within the system, and \mathbf{J} the current density. In general the current receives contributions from the free carriers, from the magnetic moments and from bound charges, so that its expression is

$$\mathbf{J} = \mathbf{J}_{carriers} + \frac{\partial \mathbf{P}}{\partial t} + c \nabla \wedge \mathbf{M}, \quad (4.99)$$

where \mathbf{P} the polarization density of bound charges⁴ and \mathbf{M} the magnetization density. In what follows we will not take into account these two terms, unless explicitly stated.

We define the displacement field \mathbf{D} through

$$\frac{1}{c} \frac{d\mathbf{D}}{dt} = \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} + \frac{4\pi}{c} \mathbf{J}. \quad (4.100)$$

By applying ∇ on both sides we get

$$\frac{1}{c} \frac{d}{dt} \nabla \cdot \mathbf{D} = \frac{1}{c} \frac{\partial}{\partial t} \nabla \cdot \mathbf{E} + \frac{4\pi}{c} \nabla \cdot \mathbf{J} = \frac{4\pi}{c} \left[\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} \right] = 0, \quad (4.101)$$

⁴The macroscopic charge density is assumed to be the average of the microscopic one over a volume element much bigger than the unit cell and smaller than the coherent volume of the applied electromagnetic field. It is reasonable to assume that, at equilibrium, this reference volume can be taken to be neutral, so that the charge density vanishes but eventually for the presence of a finite polarization \mathbf{P} and of higher multipolar components which derive from the shape of the bound-charge density. Away from equilibrium, the charge density can change also because free electrons can move or because external charges are added. Hence, neglecting higher multipoles than the dipole, the generic macroscopic charge density is

$$\rho(\mathbf{x}) = \rho_{free}(\mathbf{x}) - \nabla \cdot \mathbf{P}(\mathbf{x}) + \rho_{ext}(\mathbf{x}),$$

where ρ_{free} is the variation of the free-charge density with respect to equilibrium. The distinction between free and bound charges is however a bit matter of convention. Indeed, at frequencies much bigger than the atomic excitation ones, there is actually no distinction among them. The convention that is usually adopted, which we adopt here as well, is that the frequencies under consideration will always be much smaller than atomic ones.

where we made use of the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0.$$

We can therefore assume

$$\nabla \cdot \mathbf{D} = 0. \quad (4.102)$$

If there is an external charge with density, then (4.101) becomes

$$\frac{1}{c} \frac{d}{dt} \nabla \cdot \mathbf{D} = \frac{4\pi}{c} \frac{d\rho_{ext}}{dt},$$

implying

$$\nabla \cdot \mathbf{D} = 4\pi \rho_{ext}. \quad (4.103)$$

In other words the displacement field is only sensible to the external charge.

In the following we assume that the system is translationally invariant. In this case we can formally write a relationship between the Fourier components of \mathbf{D} , $\mathbf{D}(\omega, \mathbf{q})$, and those of \mathbf{E} , $\mathbf{E}(\omega, \mathbf{q})$:

$$\mathbf{D}(\omega, \mathbf{q}) = \epsilon(\omega, \mathbf{q}) \mathbf{E}(\omega, \mathbf{q}), \quad (4.104)$$

where $\epsilon(\omega, \mathbf{q})$ is the dielectric constant, which is actually a matrix acting on the space components, i.e. $D_i = \epsilon_{ij} E_j$ with $i, j = 1, 2, 3$. If the system is isotropic, we can generally write

$$\epsilon_{ij}(\omega, \mathbf{q}) = \frac{q_i q_j}{q^2} \epsilon_{||}(\omega, \mathbf{q}) + \left(\delta_{ij} - \frac{q_i q_j}{q^2} \right) \epsilon_{\perp}(\omega, \mathbf{q}), \quad (4.105)$$

where $\epsilon_{||}(\omega, \mathbf{q})$ is the longitudinal component of the dielectric constant and $\epsilon_{\perp}(\omega, \mathbf{q})$ the transverse one. Analogously, for any vector $\mathbf{V}(\omega, \mathbf{q})$ one can define the longitudinal component through

$$\mathbf{q} \cdot \mathbf{V}(\omega, \mathbf{q}) = q V_{||}(\omega, \mathbf{q}),$$

as well as the transverse one

$$\mathbf{V}_{\perp}(\omega, \mathbf{q}) = \mathbf{V}(\omega, \mathbf{q}) - \frac{\mathbf{q}}{q} V_{||}(\omega, \mathbf{q}).$$

In the presence of the electromagnetic field the Hamiltonian $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{Coul}$, where \mathcal{H}_0 is the kinetic energy while \mathcal{H}_{Coul} includes the electron-electron, electron-ion and ion-ion Coulomb interaction, changes according to

$$\mathcal{H}_0 \rightarrow \sum_{\sigma} \int d\mathbf{x} \frac{1}{2m} \Psi_{\sigma}(\mathbf{x})^{\dagger} \left(-i\hbar \nabla + \frac{e}{c} \mathbf{A}(\mathbf{x}) \right)^2 \Psi_{\sigma}(\mathbf{x}) - e\phi(\mathbf{x}) \Psi_{\sigma}(\mathbf{x})^{\dagger} \Psi_{\sigma}(\mathbf{x}). \quad (4.106)$$

Since we already includes the Coulomb interaction among the internal charges inside \mathcal{H}_{Coul} , the displacement, electric and magnetic fields are, in terms of the vector and scalar potentials,

$$\mathbf{D}_{||} = -\nabla\phi - \frac{1}{c}\frac{\partial}{\partial t}\mathbf{A}_{||}, \quad (4.107)$$

$$\mathbf{E}_{\perp} = -\frac{1}{c}\frac{\partial}{\partial t}\mathbf{A}_{\perp}, \quad (4.108)$$

$$\mathbf{B} = \nabla \wedge \mathbf{A}_{\perp}. \quad (4.109)$$

In other words the scalar potential and the longitudinal component of the vector potential are related only to the displacement field, which is in turn determined by the external charge through

$$\nabla \cdot \mathbf{D}_{||} = 4\pi\rho_{ext}.$$

Therefore ϕ and $\mathbf{A}_{||}$ are actually the external fields ϕ_{ext} and $\mathbf{A}_{||ext}$ applied on the system. Notice that, since only $\mathbf{D}_{||}$ has physical meaning there is a redundancy in having both ϕ and $\mathbf{A}_{||}$. This is a manifestation of the so-called gauge invariance. On the contrary, since we do not include the relativistic current-current interaction among the internal charges, the transverse electric and magnetic fields are those actually felt by the electrons inside the sample, so called internal fields.

We conclude by noticing that, in the presence of a vector potential, the charge current operator as obtained through the continuity equation

$$\frac{\partial\rho}{\partial t} + \nabla \cdot \mathbf{J} = 0,$$

changes according to

$$\begin{aligned} \mathbf{J}(\mathbf{x}) &= -e \sum_{\sigma} \left[-i\frac{\hbar}{m} \Psi_{\sigma}(\mathbf{x})^{\dagger} \nabla \Psi_{\sigma}(\mathbf{x}) + \frac{e}{mc} \Psi_{\sigma}(\mathbf{x})^{\dagger} \Psi_{\sigma}(\mathbf{x}) \mathbf{A}(\mathbf{x}, t) \right] \\ &\equiv -e\mathbf{j}(\mathbf{x}) - \frac{e^2}{mc} \rho(\mathbf{x}) \mathbf{A}(\mathbf{x}, t), \end{aligned} \quad (4.110)$$

where we defined as $-e\mathbf{j}(\mathbf{x})$ the purely electronic current, while the last term is commonly referred to as the diamagnetic term.

If we take into account also the Zeeman splitting, the Hamiltonian further contains the term

$$g\mu_B \sum_{\alpha\beta} \int d\mathbf{x} \mathbf{B}(\mathbf{x}, t) \cdot \Psi_{\alpha}(\mathbf{x})^{\dagger} \mathbf{S}_{\alpha\beta} \Psi_{\beta}(\mathbf{x}) = g\mu_B \int d\mathbf{x} \mathbf{A}_{\perp}(\mathbf{x}, t) \cdot \nabla \wedge \boldsymbol{\sigma}(\mathbf{x}), \quad (4.111)$$

where

$$\boldsymbol{\sigma}(\mathbf{x}) = \sum_{\alpha\beta} \Psi_{\alpha}(\mathbf{x})^{\dagger} \mathbf{S}_{\alpha\beta} \Psi_{\beta}(\mathbf{x}),$$

is the spin density operator, being \mathbf{S} the spin-1/2 matrices. The Zeeman splitting contributes to the current with the transverse term⁵

$$\delta\mathbf{J}(\mathbf{x}) = -c g \mu_B \nabla \wedge \boldsymbol{\sigma}(\mathbf{x}). \quad (4.112)$$

4.6.1 Response to an external charge

Let us start by studying the response to an external charge density $e \rho_{ext}(\mathbf{x}, t)$. For simplicity we will represent the ions as an infinitely massive uniform background of positive charge which has only the effect of neutralizing on average the electronic charge. In other words, if $e n$ is the charge density of the background and $\hat{\rho}(\mathbf{x})$ the density operator for the electrons, then

$$\int d\mathbf{x} \langle \hat{\rho}(\mathbf{x}) \rangle \equiv \rho(\mathbf{q} = \mathbf{0}) = V n,$$

where V is the sample volume and $\rho(\mathbf{q})$ the Fourier transform of the density. Notice that the operator $\hat{\rho}(\mathbf{q} = \mathbf{0})$ is the total number of electrons, which is conserved, hence we can always write $\hat{\rho}(\mathbf{q} = \mathbf{0}) = V n$.

If we choose a gauge in which $\mathbf{A}_{||} = 0$, the coupling to the scalar potential $\phi(\mathbf{x}, t)$ leads to the perturbation

$$\begin{aligned} \delta\hat{H} &= - \int d\mathbf{x} d\mathbf{y} \frac{e^2}{|\mathbf{x} - \mathbf{y}|} \rho_{ext}(\mathbf{x}, t) (\hat{\rho}(\mathbf{y}) - n) \\ &= -\frac{1}{V} \sum_{\mathbf{q}} \frac{4\pi e^2}{q^2} \rho_{ext}(\mathbf{q}, t) (\hat{\rho}(-\mathbf{q}) - V n \delta_{\mathbf{q}, 0}) \\ &= -\frac{1}{V} \sum_{\mathbf{q} \neq 0} \frac{4\pi e^2}{q^2} \rho_{ext}(\mathbf{q}, t) \hat{\rho}(-\mathbf{q}) \equiv -e \frac{1}{V} \sum_{\mathbf{q} \neq 0} \phi(\mathbf{q}, t) \hat{\rho}(-\mathbf{q}), \end{aligned} \quad (4.113)$$

since the Fourier transform of the scalar potential is

$$\phi(\mathbf{q}, t) = \frac{4\pi e}{q^2} \rho_{ext}(\mathbf{q}, t).$$

In the absence of the external charge, the electron density is uniform hence

$$\langle \hat{\rho}(\mathbf{y}) \rangle = n.$$

⁵Notice that the expression of the current can be also determined through the functional derivative

$$\mathbf{J}(\mathbf{x}, t) = -c \frac{\delta \mathcal{H}}{\delta \mathbf{A}(\mathbf{x}, t)}.$$

The external charge induces a deviation of the electron density with respect to the unperturbed value n , which we denote as the induced charge

$$\langle \hat{\rho}(\mathbf{y}) \rangle - n = \rho_{ind}(\mathbf{y}, t). \quad (4.114)$$

Its Fourier transform is, for $\mathbf{q} \neq \mathbf{0}$,

$$\rho_{ind}(\mathbf{q}, t) = \langle \hat{\rho}(\mathbf{q}) \rangle,$$

while for $\mathbf{q} = \mathbf{0}$ it vanishes for charge conservation. The induced charge density at frequency ω is given, within linear response theory, by

$$\rho_{ind}(\mathbf{q}, \omega) = -e\chi(\mathbf{q}, \omega)\phi(\mathbf{q}, \omega) = -\frac{4\pi e^2}{q^2}\chi(\mathbf{q}, \omega)\rho_{ext}(\mathbf{q}, \omega), \quad (4.115)$$

where

$$\chi(\mathbf{q}, \omega) = \frac{1}{V} \int_{-\infty}^{\infty} dt e^{i\omega t} (-i\theta(t)\langle [\hat{\rho}(\mathbf{q}, t), \hat{\rho}(-\mathbf{q})] \rangle), \quad (4.116)$$

is the Fourier transform of the density-density linear response function. Commonly it is denoted as the **improper** density-density linear response function, as opposed to the **proper** one which is defined through

$$\rho_{ind}(\mathbf{q}, \omega) = -\frac{4\pi e^2}{q^2}\tilde{\chi}(\mathbf{q}, \omega)(\rho_{ext}(\mathbf{q}, \omega) - \rho_{ind}(\mathbf{q}, \omega)). \quad (4.117)$$

The proper function gives the response of the electrons to the internal field, which is generated both by the external charge and by the same electrons.⁶ Comparing (4.115) with (4.117) we find that

$$\chi(\mathbf{q}, \omega) = \frac{\tilde{\chi}(\mathbf{q}, \omega)}{1 - \frac{4\pi e^2}{q^2}\tilde{\chi}(\mathbf{q}, \omega)}. \quad (4.118)$$

By definition

$$\begin{aligned} i\mathbf{q} \cdot \mathbf{D}_{||}(\mathbf{q}, \omega) &\equiv i\mathbf{q} \cdot \epsilon_{||}(\mathbf{q}, \omega)\mathbf{E}_{||}(\mathbf{q}, \omega) = 4\pi e\rho_{ext}(\mathbf{q}, \omega), \\ i\mathbf{q} \cdot \mathbf{E}_{||}(\mathbf{q}, \omega) &= 4\pi e\rho_{ext}(\mathbf{q}, \omega) - 4\pi e\rho_{ind}(\mathbf{q}, \omega), \end{aligned}$$

hence

$$\epsilon_{||}(\mathbf{q}, \omega)(\rho_{ext}(\mathbf{q}, \omega) - \rho_{ind}(\mathbf{q}, \omega)) = \rho_{ext}(\mathbf{q}, \omega).$$

In other words

$$\frac{1}{\epsilon_{||}(\mathbf{q}, \omega)} = 1 - \frac{\rho_{ind}(\mathbf{q}, \omega)}{\rho_{ext}(\mathbf{q}, \omega)}, \quad (4.119)$$

⁶The induced charge refers to electrons, which explains the minus sign in (4.117)

$$\epsilon_{||}(\mathbf{q}, \omega) = 1 + \frac{\rho_{ind}(\mathbf{q}, \omega)}{\rho_{ext}(\mathbf{q}, \omega) - \rho_{ind}(\mathbf{q}, \omega)}. \quad (4.120)$$

Through Eqs. (4.115) and (4.119) it derives that

$$\frac{1}{\epsilon_{||}(\mathbf{q}, \omega)} = 1 + \frac{4\pi e^2}{q^2} \chi(\mathbf{q}, \omega), \quad (4.121)$$

while by the Eqs. (4.117) and (4.120)

$$\epsilon_{||}(\mathbf{q}, \omega) = 1 - \frac{4\pi e^2}{q^2} \tilde{\chi}(\mathbf{q}, \omega). \quad (4.122)$$

These two equations relate the longitudinal dielectric constant to the density-density proper and improper response functions. Notice that for the dielectric constant the Kramers-Krönig relations read

$$\mathcal{R}e \frac{1}{\epsilon_{||}(\mathbf{q}, \omega)} = 1 - \mathcal{P} \int \frac{d\omega'}{\pi} \frac{1}{\omega - \omega'} \mathcal{I}m \frac{1}{\epsilon_{||}(\mathbf{q}, \omega')}. \quad (4.123)$$

Using once more the definition of the displacement field, one finds that

$$\frac{d}{dt} \nabla \cdot \mathbf{D} = \partial_t \nabla \cdot \mathbf{E} + 4\pi \nabla \cdot \mathbf{J},$$

where \mathbf{J} is the current flowing inside the system.⁷ In Fourier space it reads

$$q\omega D_{||}(\mathbf{q}, \omega) = q\omega E_{||}(\mathbf{q}, \omega) + 4\pi i \mathbf{q} \cdot \mathbf{J}(\mathbf{q}, \omega).$$

Since $D_{||} = \epsilon_{||} E_{||}$, we find

$$J_{||}(\mathbf{q}, \omega) = \frac{\omega}{4\pi i} (\epsilon_{||}(\mathbf{q}, \omega) - 1) E_{||}(\mathbf{q}, \omega) \equiv \sigma_{||}(\mathbf{q}, \omega) E_{||}(\mathbf{q}, \omega),$$

where $\sigma_{||}$ is the longitudinal conductivity which relates the current to the internal electric field. Therefore

$$\sigma_{||}(\mathbf{q}, \omega) = \frac{\omega}{4\pi i} (\epsilon_{||}(\mathbf{q}, \omega) - 1), \quad (4.124)$$

$$\epsilon_{||}(\mathbf{q}, \omega) = 1 + \frac{4\pi i}{\omega} \sigma_{||}(\mathbf{q}, \omega). \quad (4.125)$$

⁷Since we assumed an external probing charge $\rho_{ext}(\mathbf{x}, t)$ which depends on time only explicitly, the total flowing current includes just the induced one.

Gauge invariance and its consequences

So far we have adopted a gauge where the external scalar field is finite while the external longitudinal vector potential is zero. Now let us do the opposite, keeping the physical displacement field fixed. By gauge invariance the response of the system should be the same. Therefore let us consider an external charge density $e\rho_{ext}(\mathbf{x}, t)$ leading to a displacement field

$$D_{||}(\mathbf{q}, \omega) = \frac{e}{iq} \rho_{ext}(\mathbf{q}, \omega).$$

We assume that

$$D_{||}(\mathbf{q}, \omega) = \frac{i\omega}{c} A_{||}(\mathbf{q}, \omega) = \epsilon_{||}(\mathbf{q}, \omega) E_{||}(\mathbf{q}, \omega).$$

A vector potential provides a perturbation

$$\delta\mathcal{H} = \frac{e}{c} \int d\mathbf{x} \mathbf{A}(\mathbf{x}, t) \cdot \mathbf{j}(\mathbf{x}) + \frac{e^2}{2mc^2} \int d\mathbf{x} \rho(\mathbf{x}) \mathbf{A}(\mathbf{x}, t) \cdot \mathbf{A}(\mathbf{x}, t), \quad (4.126)$$

where the electronic current \mathbf{j} has been defined by Eq. (4.110) and $\rho(\mathbf{x}) = \sum_\sigma \Psi_\sigma(\mathbf{x})^\dagger \Psi_\sigma(\mathbf{x})$ is the density operator. The longitudinal value of \mathbf{j} is given in linear response by

$$j_{||}(\mathbf{q}, \omega) = \frac{e}{c} \chi_{||}(\mathbf{q}, \omega) A_{||}(\mathbf{q}, \omega),$$

where, if

$$\chi_{lm}(\mathbf{x}, t) = -i\theta(t) \langle [\mathbf{j}_l(\mathbf{x}, t), \mathbf{j}_m(\mathbf{0}, 0)] \rangle$$

is the current-current response function, then its longitudinal component is defined through

$$\chi_{||}(\mathbf{q}, \omega) = \sum_{lm} \int dt e^{i\omega t} \int d\mathbf{x} e^{-i\mathbf{q}\cdot\mathbf{x}} \frac{q_l q_m}{q^2} \chi_{lm}(\mathbf{x}, t).$$

On the other hand the true charge current operator, see Eq. (4.110), is

$$\mathbf{J}(\mathbf{x}, t) = -e\mathbf{j}(\mathbf{x}, t) - \frac{e^2}{mc} \langle \rho(\mathbf{x}) \rangle \mathbf{A}_{||}(\mathbf{x}, t).$$

Since the second term in the right hand side is already linear in the external field, the average of the density operator has to be evaluated on the unperturbed state, where $\langle \rho(\mathbf{x}) \rangle = n$. Hence

$$\begin{aligned} J_{||}(\mathbf{q}, \omega) &= -ej_{||}(\mathbf{q}, \omega) - \frac{ne^2}{mc} A_{||}(\mathbf{q}, \omega) \\ &= -\frac{e^2}{c} \left(\chi_{||}(\mathbf{q}, \omega) + \frac{n}{m} \right) A_{||}(\mathbf{q}, \omega) \\ &= -\frac{e^2}{i\omega} \left(\chi_{||}(\mathbf{q}, \omega) + \frac{n}{m} \right) \epsilon_{||}(\mathbf{q}, \omega) E_{||}(\mathbf{q}, \omega) \equiv \sigma_{||}(\mathbf{q}, \omega) E_{||}(\mathbf{q}, \omega). \end{aligned}$$

Therefore we find that

$$\sigma_{||}(\mathbf{q}, \omega) = -\frac{e^2}{i\omega} \left(\chi_{||}(\mathbf{q}, \omega) + \frac{n}{m} \right) \epsilon_{||}(\mathbf{q}, \omega),$$

which, compared with (4.124) leads to

$$-\frac{e^2}{i\omega} \left(\chi_{||}(\mathbf{q}, \omega) + \frac{n}{m} \right) \epsilon_{||}(\mathbf{q}, \omega) = \frac{\omega}{4\pi i} (\epsilon_{||}(\mathbf{q}, \omega) - 1),$$

namely

$$\begin{aligned} \chi_{||}(\mathbf{q}, \omega) + \frac{n}{m} &= -\frac{\omega^2}{4\pi e^2} \left(1 - \frac{1}{\epsilon_{||}(\mathbf{q}, \omega)} \right) \\ &= \frac{\omega^2}{q^2} \chi(\mathbf{q}, \omega). \end{aligned} \quad (4.127)$$

This shows that gauge invariance implies that the longitudinal current-current response function can be expressed in terms of the density-density response function.

In principle we can also introduce a proper longitudinal current-current response function through

$$\begin{aligned} J_{||}(\mathbf{q}, \omega) &= -\frac{e^2}{i\omega} \left(\chi_{||}(\mathbf{q}, \omega) + \frac{n}{m} \right) \epsilon_{||}(\mathbf{q}, \omega) E_{||}(\mathbf{q}, \omega) \\ &\equiv -\frac{e^2}{i\omega} \left(\widetilde{\chi}_{||}(\mathbf{q}, \omega) + \frac{n}{m} \right) E_{||}(\mathbf{q}, \omega), \end{aligned}$$

which is related by gauge invariance to the proper density-density response function through

$$q^2 \left(\widetilde{\chi}_{||}(\mathbf{q}, \omega) + \frac{n}{m} \right) = \omega^2 \widetilde{\chi}(\mathbf{q}, \omega). \quad (4.128)$$

We end by noticing that, in the gauge in which the scalar potential is zero, the internal longitudinal vector potential, defined by

$$A_{|| int}(\mathbf{q}, \omega) = \frac{c}{i\omega} E_{||}(\mathbf{q}, \omega),$$

is related to the external one,

$$A_{||}(\mathbf{q}, \omega) = A_{|| ext}(\mathbf{q}, \omega) = \frac{c}{i\omega} D_{||}(\mathbf{q}, \omega),$$

through

$$A_{|| int}(\mathbf{q}, \omega) = \frac{1}{\epsilon_{||}(\mathbf{q}, \omega)} A_{|| ext}(\mathbf{q}, \omega). \quad (4.129)$$

4.6.2 Response to a transverse field

By recalling the definition of the displacement field

$$\frac{d}{dt} \mathbf{D} = \partial_t \mathbf{E} + 4\pi \mathbf{J},$$

its transverse component is given by

$$\begin{aligned} -i\omega D_{\perp}(\mathbf{q}, \omega) &= -i\omega \epsilon_{\perp}(\mathbf{q}, \omega) E_{\perp}(\mathbf{q}, \omega) = -i\omega E_{\perp}(\mathbf{q}, \omega) + 4\pi J_{\perp}(\mathbf{q}, \omega) \\ &= (-i\omega + 4\pi \sigma_{\perp}(\mathbf{q}, \omega)) E_{\perp}(\mathbf{q}, \omega), \end{aligned}$$

which provides the relationship between the transverse dielectric constant and conductivity:

$$\epsilon_{\perp}(\mathbf{q}, \omega) = 1 + \frac{4\pi i}{\omega} \sigma_{\perp}(\mathbf{q}, \omega). \quad (4.130)$$

We already said that the transverse vector potential is actually the internal one, so the response to it is connected with proper response functions. Following the same reasoning as after Eq. (4.126) but now for the transverse current, we get to the conclusion that

$$\mathbf{J}_{\perp}(\mathbf{q}, \omega) = -\frac{e^2}{c} \left(\tilde{\chi}_{\perp}(\mathbf{q}, \omega) + \frac{n}{m} \right) A_{\perp}(\mathbf{q}, \omega), \quad (4.131)$$

where $\tilde{\chi}_{\perp}(\mathbf{q}, \omega)$ is obtained by the current-current response function through

$$\chi_{lm}(\mathbf{q}, \omega) = \frac{q_l q_m}{q^2} \chi_{||}(\mathbf{q}, \omega) + \left(\delta_{lm} - \frac{q_l q_m}{q^2} \right) \tilde{\chi}_{\perp}(\mathbf{q}, \omega). \quad (4.132)$$

Notice that, unlike the longitudinal one, the transverse component is proper. Since

$$J_{\perp}(\mathbf{q}, \omega) = \sigma_{\perp} E_{\perp}(\mathbf{q}, \omega) = \frac{i\omega}{c} \sigma_{\perp} A_{\perp}(\mathbf{q}, \omega), \quad (4.133)$$

we finally obtain

$$\sigma_{\perp}(\mathbf{q}, \omega) = -\frac{e^2}{i\omega} \left(\tilde{\chi}_{\perp}(\mathbf{q}, \omega) + \frac{n}{m} \right). \quad (4.134)$$

By means of (4.108) and (4.109) and the last Maxwell equation we get the usual wave-equation for the internal vector potential

$$-\nabla^2 \mathbf{A}_{\perp} = -\frac{1}{c^2} \frac{\partial^2 \mathbf{A}_{\perp}}{\partial t^2} + \frac{4\pi}{c} \mathbf{J}_{\perp tot},$$

which in momentum and frequency space reads

$$(c^2 q^2 - \omega^2) \mathbf{A}_{\perp}(\mathbf{q}, \omega) = 4\pi c \mathbf{J}_{\perp tot}(\mathbf{q}, \omega). \quad (4.135)$$

The current appearing in (4.135) is the total one, including the external source of the electromagnetic field. The latter satisfies a similar equation

$$(c^2 q^2 - \omega^2) \mathbf{A}_{\perp ext}(\mathbf{q}, \omega) = 4\pi c \mathbf{J}_{\perp ext}(\mathbf{q}, \omega),$$

in terms of the external current source. Writing $\mathbf{J}_{\perp tot} = \mathbf{J}_{\perp ext} + \mathbf{J}_{\perp}$, with the latter being the induced current as given by (4.133), we finally get

$$(c^2 q^2 - \omega^2) \mathbf{A}_{\perp}(\mathbf{q}, \omega) = (c^2 q^2 - \omega^2) \mathbf{A}_{\perp ext}(\mathbf{q}, \omega) + 4\pi i \omega \sigma_{\perp}(\mathbf{q}, \omega) \mathbf{A}_{\perp}(\mathbf{q}, \omega).$$

In other words, the internal vector potential, $\mathbf{A}_{\perp} = \mathbf{A}_{\perp int}$, is related to the applied one by the equation

$$\begin{aligned} \mathbf{A}_{\perp int}(\mathbf{q}, \omega) &= \frac{c^2 q^2 - \omega^2}{c^2 q^2 - \omega^2 - 4\pi i \omega \sigma_{\perp}(\mathbf{q}, \omega)} \mathbf{A}_{\perp ext}(\mathbf{q}, \omega) \\ &= \frac{c^2 q^2 - \omega^2}{c^2 q^2 - \omega^2 \epsilon_{\perp}(\mathbf{q}, \omega)} \mathbf{A}_{\perp ext}(\mathbf{q}, \omega), \end{aligned} \quad (4.136)$$

to be compared with (4.129) valid for the longitudinal component.

Let us introduce back the Zeeman contribution to the transverse current given in Eq. (4.112). Within linear response theory and assuming a uniform isotropic system

$$\boldsymbol{\sigma}(\mathbf{x}, t) = g\mu_B \int d\mathbf{y} dt' \chi_{\sigma}(\mathbf{x} - \mathbf{y}, t - t') \mathbf{B}(\mathbf{y}, t') = g\mu_B \int d\mathbf{y} dt' \chi_{\sigma}(\mathbf{x} - \mathbf{y}, t - t') \nabla_{\mathbf{y}} \wedge \mathbf{A}_{\perp}(\mathbf{y}, t'),$$

where χ_{σ} is the spin-density response function. Therefore (4.112) is, at linear order,

$$\begin{aligned} \delta \mathbf{J}(\mathbf{x}) &= -c(g\mu_B)^2 \int d\mathbf{y} dt' \nabla_{\mathbf{x}} \wedge [\chi_{\sigma}(\mathbf{x} - \mathbf{y}, t - t') \nabla_{\mathbf{y}} \wedge \mathbf{A}_{\perp}(\mathbf{y}, t')] \\ &= c(g\mu_B)^2 \int d\mathbf{y} dt' \nabla^2 \chi_{\sigma}(\mathbf{x} - \mathbf{y}, t - t') \mathbf{A}_{\perp}(\mathbf{y}, t'), \end{aligned} \quad (4.137)$$

which, after Fourier transform, is

$$\delta \mathbf{J}_{\perp}(\mathbf{q}, \omega) = -c q^2 (g\mu_B)^2 \chi_{\sigma}(\mathbf{q}, \omega) \mathbf{A}_{\perp}(\mathbf{q}, \omega).$$

This term modifies (4.136) into

$$\mathbf{A}_{\perp int}(\mathbf{q}, \omega) = \frac{c^2 q^2 - \omega^2}{c^2 q^2 - \omega^2 \epsilon_{\perp}(\mathbf{q}, \omega) + 4\pi c^2 q^2 (g\mu_B)^2 \chi_{\sigma}(\mathbf{q}, \omega)} \mathbf{A}_{\perp ext}(\mathbf{q}, \omega). \quad (4.138)$$

4.6.3 Limiting values of the response functions

The values of the response functions in some particular limits of physical significance can be obtained without making any complicated calculation.

Consequences of the f -sum rule

The charge density operator at $\mathbf{q} = \mathbf{0}$ is the total number of electrons N , which is a conserved quantity, independent upon time. Therefore

$$\chi(\mathbf{q} = \mathbf{0}, t) = -i \frac{1}{V} \theta(t) \langle [\hat{\rho}(\mathbf{0}, t), \hat{\rho}(\mathbf{0})] \rangle = -i \frac{1}{V} \theta(t) \langle [N, N] \rangle = 0.$$

In other words due to charge conservation it holds that

$$\boxed{\chi(\mathbf{0}, \omega) = 0}. \quad (4.139)$$

The dissipative density-density response function is by definition

$$\chi''(\mathbf{q}, t) = \frac{1}{2V} \langle [\hat{\rho}(\mathbf{q}, t), \hat{\rho}(-\mathbf{q})] \rangle = \int \frac{d\omega}{2\pi} e^{-i\omega t} \chi''(\mathbf{q}, \omega).$$

By means of the continuity equation

$$\begin{aligned} i \frac{\partial \chi''(\mathbf{q}, t)}{\partial t} &= \frac{1}{2V} \left\langle \left[i \frac{\partial \hat{\rho}(\mathbf{q}, t)}{\partial t}, \hat{\rho}(-\mathbf{q}) \right] \right\rangle \\ &= \frac{1}{2V} \langle [\mathbf{q} \cdot \mathbf{J}(\mathbf{q}, t), \hat{\rho}(-\mathbf{q})] \rangle \\ &= \int \frac{d\omega}{2\pi} e^{-i\omega t} \omega \chi''(\mathbf{q}, \omega). \end{aligned}$$

On the other hand, for $t = 0$, the following expression holds

$$\frac{1}{2V} \langle [\mathbf{q} \cdot \mathbf{J}(\mathbf{q}), \hat{\rho}(-\mathbf{q})] \rangle = \frac{nq^2}{2m},$$

which leads to the so-called f -sum rule

$$\int \frac{d\omega}{2\pi} \omega \chi''(\mathbf{q}, \omega) = \frac{nq^2}{2m}. \quad (4.140)$$

By the Kramers-Kronig relations

$$\mathcal{R}e \chi(\mathbf{q}, \omega) = \mathcal{P} \int \frac{d\omega'}{\pi} \frac{\chi''(\mathbf{q}, \omega')}{\omega - \omega'}.$$

We know that the dissipative response function is finite only for frequencies which correspond to the energies of excitations which may be created by the density operators. In other words $\chi''(\mathbf{q}, \omega')$ is bounded from above. Therefore if we consider a frequency much above this upper

bound, and we recall that the dissipative response function is odd in frequency, then we find that

$$\begin{aligned}\lim_{\omega \rightarrow \infty} \mathcal{R}e \chi(\mathbf{q}, \omega) &= \int \frac{d\omega'}{\pi} \frac{\chi''(\mathbf{q}, \omega')}{\omega} \left(1 + \frac{\omega'}{\omega}\right) \\ &= \frac{1}{\omega^2} \int \frac{d\omega'}{\pi} \omega' \chi''(\mathbf{q}, \omega') = \frac{nq^2}{m\omega^2},\end{aligned}$$

namely

$$\boxed{\lim_{\omega \rightarrow \infty} \mathcal{R}e \chi(\mathbf{q}, \omega) = \frac{nq^2}{m\omega^2}}. \quad (4.141)$$

Alternatively, we can re-write the sum-rule (4.140) as

$$\begin{aligned}\frac{n}{2m} &= \frac{1}{q^2} \int \frac{d\omega'}{2\pi} \omega' \chi''(\mathbf{q}, \omega') = -\frac{1}{q^2} \int \frac{d\omega'}{2\pi} \omega' \mathcal{I}m \chi(\mathbf{q}, \omega') \\ &= - \int \frac{d\omega'}{2\pi} \frac{1}{\omega'} \mathcal{I}m \left(\chi_{||}(\mathbf{q}, \omega') + \frac{n}{m} \right).\end{aligned}$$

In the limit $\mathbf{q} \rightarrow \mathbf{0}$, there is no distinction between longitudinal and transverse response, so that, through Eq. (4.132), we obtain

$$\begin{aligned}\frac{n}{2m} &= - \lim_{\mathbf{q} \rightarrow \mathbf{0}} \int \frac{d\omega'}{2\pi} \frac{1}{\omega'} \mathcal{I}m \left(\chi_{||}(\mathbf{q}, \omega') + \frac{n}{m} \right) \\ &= - \lim_{\mathbf{q} \rightarrow \mathbf{0}} \int \frac{d\omega'}{2\pi} \frac{1}{\omega'} \mathcal{I}m \left(\tilde{\chi}_{\perp}(\mathbf{q}, \omega') + \frac{n}{m} \right) \\ &= \int \frac{d\omega'}{2\pi} \mathcal{I}m \left(\frac{i}{e^2} \sigma_{\perp}(\mathbf{0}, \omega') \right).\end{aligned}$$

In other words, the f -sum rule can also be written as

$$\boxed{\int_0^\infty d\omega \mathcal{R}e \sigma_{\perp}(\mathbf{0}, \omega) = \frac{ne^2}{2m}}, \quad (4.142)$$

which is the so-called optical f -sum rule.

By Eq. (4.121) we also find that

$$\boxed{\lim_{\omega \rightarrow \infty} \mathcal{R}e \frac{1}{\epsilon_{||}(\mathbf{q}, \omega)} = 1 + \frac{\omega_p^2}{\omega^2}}, \quad (4.143)$$

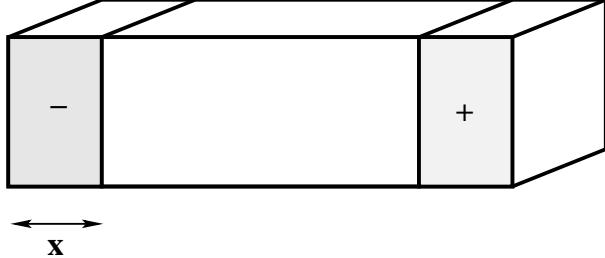


Figure 4.1: Pictorial representation of a plasmon excitation.

as well as

$$\boxed{\int \frac{d\omega'}{\pi} \omega' \mathcal{I}m \frac{1}{\epsilon_{||}(\mathbf{q}, \omega')} = -\omega_p^2}, \quad (4.144)$$

where

$$\omega_p = \sqrt{\frac{4\pi n e^2}{m}} \quad (4.145)$$

is the so-called electron **plasma frequency**.

What is the meaning of the plasma frequency? Let us take a piece of metal and let us displace uniformly, *i.e.* at $\mathbf{q} = \mathbf{0}$, the valence electrons with respect to the positive background⁸ by a distance x , as in Fig. 4.1. As a result a surface charge will appear $\sigma = n e x$, so that x is subject to a restoring Coulomb force

$$m \frac{d^2 x}{dt^2} = -4\pi e \sigma = -4\pi e^2 n x, \quad (4.146)$$

leading to oscillations, so-called plasmons, with frequency ω_p . In other words the only longitudinal modes at $\mathbf{q} = \mathbf{0}$ allowed in a metal are plasmons. Taking into account (4.144), which is valid for all q 's, hence also for $q \rightarrow 0$, we conclude that

$$\lim_{q \rightarrow 0} \mathcal{I}m \frac{1}{\epsilon_{||}(\mathbf{q}, \omega)} = -\frac{\pi}{2} \omega_p (\delta(\omega - \omega_p) - \delta(\omega + \omega_p)), \quad (4.147)$$

which, by Kramer-Krönig transformation, leads to

$$\boxed{\mathcal{R}e \frac{1}{\epsilon_{||}(\mathbf{0}, \omega)} = \frac{\omega^2}{\omega^2 - \omega_p^2}},$$

⁸In a real solid we have to imagine that the positive background includes the ions and the bound electrons. In other words the derivation implicitly assumes that we explore excitations at frequency smaller than interband transitions.

or, equivalently,

$$\frac{1}{\epsilon_{||}(\mathbf{0}, \omega)} = 1 + \frac{\omega_p}{2} \left(\frac{1}{\omega - \omega_p + i\eta} - \frac{1}{\omega + \omega_p + i\eta} \right), \quad (4.148)$$

with η an infinitesimal positive number. In addition

$$\operatorname{Re} \epsilon_{||}(\mathbf{0}, \omega) = 1 - \frac{\omega_p^2}{\omega^2}.$$

Through (4.122) we also find that

$$\lim_{q \rightarrow 0} \tilde{\chi}(\mathbf{q}, \omega) = \frac{n}{m} \frac{q^2}{\omega^2}, \quad (4.149)$$

which, through the gauge relation (4.128), leads to

$$\lim_{q \rightarrow 0} \widetilde{\chi}_{||}(\mathbf{q}, \omega) = 0. \quad (4.150)$$

Finally, using the definition of the longitudinal conductivity (4.124), we also find that

$$\operatorname{Re} \sigma_{||}(\mathbf{0}, \omega) = \operatorname{Re} i \frac{ne^2}{m} \frac{1}{\omega + i\eta} = \pi \frac{ne^2}{m} \delta(\omega),$$

which implies an infinite conductivity of an ideal metal.

Zero frequency response

Now suppose we change by the same amount the charge density of the positive background and of the electrons, for instance by changing the volume V . From the point of view of the electrons, this is analogous to changing the chemical potential, hence

$$\int d\mathbf{x} \langle \hat{\rho}(\mathbf{x}) \rangle - n = \delta N = \frac{\partial N}{\partial \mu} \delta \mu.$$

The compressibility is defined by

$$K = -\frac{1}{V} \frac{\partial V}{\partial P},$$

where P is the pressure. The free-energy $F(N, V, T)$ can be written as

$$F(N, V, T) = V f(n, T),$$

so that the pressure

$$P = -\frac{\partial F}{\partial V} = -f + n \frac{\partial f}{\partial n},$$

hence

$$\frac{1}{K} = n^2 \frac{\partial^2 f}{\partial n^2}.$$

On the other hand

$$\mu = \frac{\partial F}{\partial N} = \frac{\partial f}{\partial n}, \quad \frac{\partial \nu}{\partial N} = \frac{1}{V} \frac{\partial^2 f}{\partial n^2},$$

implying that

$$\frac{\partial N}{\partial \mu} = n^2 K V. \quad (4.151)$$

From the point of view of the Hamiltonian, the action of changing the density of the background and in the meantime changing the electron chemical potential so to maintain charge neutrality corresponds to a time-independent perturbation

$$\delta \mathcal{H} = \frac{1}{V} \sum_{\mathbf{q}} V_{ext}(-\mathbf{q}, \omega = 0) \hat{\rho}(\mathbf{q}),$$

where

$$V_{ext}(\mathbf{q}, \omega = 0) = -\frac{4\pi e^2}{q^2} \delta \rho_{back}(\mathbf{q}, \omega = 0) - V \delta \mu \delta_{\mathbf{q}, \mathbf{0}}.$$

The internal field is instead

$$V_{int}(\mathbf{q}, \omega = 0) = -\frac{4\pi e^2}{q^2} (\delta \rho_{back}(\mathbf{q}, \omega = 0) - \delta \rho_{el}(\mathbf{q}, \omega = 0)) - V \delta \mu \delta_{\mathbf{q}, \mathbf{0}},$$

and, by definition,

$$\delta \rho_{el}(\mathbf{q}, \omega = 0) = \tilde{\chi}(\mathbf{q}, \omega = 0) V_{int}(\mathbf{q}, \omega = 0).$$

Since charge neutrality is maintained, in the limit $\mathbf{q} \rightarrow \mathbf{0}$ we find

$$\lim_{\mathbf{q} \rightarrow \mathbf{0}} V_{int}(\mathbf{q}, \omega = 0) = -V \delta \mu,$$

hence

$$\lim_{\mathbf{q} \rightarrow \mathbf{0}} \delta \rho_{el}(\mathbf{q}, \omega = 0) = \delta N = -V \delta \mu \lim_{\mathbf{q} \rightarrow \mathbf{0}} \tilde{\chi}(\mathbf{q}, \omega = 0) = n^2 K V \delta \mu,$$

leading to the relationship

$$\lim_{\mathbf{q} \rightarrow \mathbf{0}} \tilde{\chi}(\mathbf{q}, 0) = -n^2 K. \quad (4.152)$$

In terms of the dielectric constant it implies that

$$\boxed{\lim_{\mathbf{q} \rightarrow 0} \epsilon_{||}(\mathbf{q}, 0) = 1 + \frac{4\pi n^2 e^2}{q^2} K \rightarrow \infty}. \quad (4.153)$$

The dielectric constant at zero frequency diverges when the momentum vanishes, provided the compressibility is finite. What is the meaning of a finite or vanishing compressibility? We have shown that

$$K = \frac{1}{n^2 V} \frac{\partial N}{\partial \mu}.$$

If the system is a metal, the number of electrons is a continuous and increasing function of the chemical potential, hence K is finite. On the contrary, if the system is an insulator, the chemical potential lies within an energy gap so that the number of electrons stays constant upon small changes of μ , implying $K = 0$. In other words a finite or vanishing compressibility discriminates between metals and insulators. Equivalently, a metal has a longitudinal dielectric constant at zero frequency which diverges as $\mathbf{q} \rightarrow \mathbf{0}$, while for an insulator this limit is finite. To better appreciate this difference, let us consider the response to an external point-like charge, for instance at position \mathbf{x}_0

$$\rho_{ext}(\mathbf{x}, t) = Z \delta(\mathbf{x} - \mathbf{x}_0), \quad \rho_{ext}(\mathbf{q}, \omega) = Z \delta(\omega) e^{-i\mathbf{q} \cdot \mathbf{x}_0}.$$

According to our definitions, the induced density is

$$\begin{aligned} \rho_{ind}(\mathbf{q}, \omega) &= -\frac{4\pi e^2}{q^2} \chi(\mathbf{q}, \omega) \rho_{ext}(\mathbf{q}, \omega) = -Z \frac{4\pi e^2}{q^2} \frac{\tilde{\chi}(\mathbf{q}, \omega)}{\epsilon_{||}(\mathbf{q}, \omega)} \delta(\omega) e^{-i\mathbf{q} \cdot \mathbf{x}_0} \\ &= Z \delta(\omega) e^{-i\mathbf{q} \cdot \mathbf{x}_0} \frac{\epsilon_{||}(\mathbf{q}, 0) - 1}{\epsilon_{||}(\mathbf{q}, 0)} = \rho_{ext}(\mathbf{q}, \omega) \frac{\epsilon_{||}(\mathbf{q}, 0) - 1}{\epsilon_{||}(\mathbf{q}, 0)}. \end{aligned}$$

Therefore the net charge inside the system is

$$e (\rho_{ext}(\mathbf{q}, \omega) - \rho_{ind}(\mathbf{q}, \omega)) = e \rho_{ext}(\mathbf{q}, \omega) \frac{1}{\epsilon_{||}(\mathbf{q}, 0)}.$$

Since $\epsilon_{||}(\mathbf{q}, 0)$ diverges for small q in a metal, then, in the same limit, the total charge inside the system vanishes, which implies that in a metal the induced charge is always such as to perfectly screen the external one,

Transverse response

We already know that

$$\lim_{\mathbf{q} \rightarrow 0} \chi_{||}(\mathbf{q}, \omega) = 0.$$

Since for $\mathbf{q} \rightarrow \mathbf{0}$ at fixed frequency there is no difference between transverse and longitudinal fields, this also implies that

$$\lim_{\mathbf{q} \rightarrow \mathbf{0}} \widetilde{\chi}_{\perp}(\mathbf{q}, \omega) = 0.$$

Through Eqs. (4.134) and (4.130) we then find

$$\lim_{\mathbf{q} \rightarrow \mathbf{0}} \sigma_{\perp}(\mathbf{q}, \omega) = -\frac{\omega_p^2}{4\pi i\omega}, \quad (4.154)$$

$$\lim_{\mathbf{q} \rightarrow \mathbf{0}} \epsilon_{\perp}(\mathbf{q}, \omega) = 1 - \frac{\omega_p^2}{\omega^2}. \quad (4.155)$$

On the other hand we also know that

$$\lim_{\mathbf{q} \rightarrow \mathbf{0}} \widetilde{\chi}(\mathbf{q}, 0) = -n^2 K,$$

so that from the gauge relation we should have

$$\lim_{\mathbf{q} \rightarrow \mathbf{0}} \widetilde{\chi}_{||}(\mathbf{q}, 0) = -\frac{n}{m}.$$

The transverse response at $\omega = 0$ is the response to a finite magnetic field in the absence of electric one, as $E_{\perp} = i\omega A_{\perp}/c$. Since the transverse conductivity is not expected to be singular in the presence of a magnetic field, we have to conclude from (4.134) that also

$$\lim_{\mathbf{q} \rightarrow \mathbf{0}} \lim_{\omega \rightarrow 0} \widetilde{\chi}_{\perp}(\mathbf{q}, \omega) = -\frac{n}{m}.$$

The approach to this limiting value should be regular, so that we expect that

$$\lim_{\mathbf{q} \rightarrow \mathbf{0}} \lim_{\omega \rightarrow 0} \widetilde{\chi}_{\perp}(\mathbf{q}, \omega) = -\frac{n}{m} \left(1 - \frac{q^2}{Ak_F^2}\right), \quad (4.156)$$

with A a dimensionless constant and k_F the Fermi momentum.⁹ Through Eq. (4.134) we then find

$$\lim_{\mathbf{q} \rightarrow \mathbf{0}} -4\pi i\omega \sigma_{\perp}(\mathbf{q}, \omega) = \omega_p^2 \frac{q^2}{Ak_F^2},$$

which inserted in (4.138) gives

$$\mathbf{A}_{\perp int}(\mathbf{q}, 0) = \frac{Ac^2 k_F^2}{Ac^2 k_F^2 + \omega_p^2 + 4\pi c^2 A k_F^2 (g\mu_B)^2 \chi_{\sigma}} \mathbf{A}_{\perp ext}(\mathbf{q}, 0), \quad (4.157)$$

⁹ $A = 4$ for free electrons

being χ_σ the magnetic susceptibility, which we know is negative. Since an $\omega = 0$ transverse vector potential corresponds to a constant magnetic field in the absence of electric one, (4.157) implies that the magnetic field can penetrate inside the metal. The Zeeman term would lead to an increased amplitude with respect to the applied one (Landau paramagnetism), while the free-carrier term to a decrease (Landau diamagnetism).¹⁰

On the contrary, since $\epsilon_{||}(\mathbf{q}, 0)$ diverges as $\mathbf{q} \rightarrow \mathbf{0}$, from (4.129) one realizes that a longitudinal field does not propagate freely inside a metal. Indeed, using Eq. (4.153), we can write

$$\epsilon_{||}(\mathbf{q}, 0) = 1 + \frac{4\pi n^2 e^2}{q^2} K f(q),$$

with $f(0) = 1$. If $f(q)$ were analytic, then through

$$A_{|| int}(\mathbf{q}, 0) = \frac{q^2}{q^2 + 4\pi n^2 e^2 K f(q)} A_{|| ext}(\mathbf{q}, 0),$$

and upon Fourier transform in real space, we would find a longitudinal vector potential decaying exponentially inside the sample, with a decay length

$$\lambda_{TF} = \frac{1}{4\pi n^2 e^2},$$

which is called the Thomas-Fermi screening length.¹¹ In reality the function $f(q)$ is non-analytic. It has a branch cut starting from $q = 2k_F$ due to the Fermi surface. The reason is that it is not possible to create a particle-hole excitation at zero-frequency if the transferred momentum $q > 2k_F$, hence the imaginary part of the density-density response function contains a step-function which turns into a log-singularity in the real part. The final result is that the longitudinal field far away from the external source decays as $\cos(2k_F r)/r^3$, so called Friedel oscillatory behavior.

4.6.4 Power dissipated by the electromagnetic field

In the presence of an external longitudinal field, the power dissipated according to the general formula is

$$W = \left(\frac{e}{c}\right)^2 \frac{\omega}{2} |A_{|| ext}(\mathbf{q}, \omega)|^2 \chi''_{||}(\mathbf{q}, \omega) = -\left(\frac{e}{c}\right)^2 \frac{\omega}{2} |A_{|| ext}(\mathbf{q}, \omega)|^2 \text{Im} \chi_{||}(\mathbf{q}, \omega)$$

¹⁰For free electrons the diamagnetic term is 1/3 of the paramagnetic one, so the field is actually enhanced within the interior of the system.

¹¹Indeed this is the same screening length one would obtain within the Thomas-Fermi approximation. Namely, if we consider the equation for the internal scalar potential in the presence of a time-independent external charge

$$\nabla^2 \phi(\mathbf{x}) = -4\pi \rho_{ext}(\mathbf{x}) - 4\pi \rho_{ind}(\mathbf{x}),$$

and we assume a very weak space-dependence so that

$$\rho_{ind}(\mathbf{x}) \simeq -\frac{e}{V} \frac{\partial N}{\partial \mu} (-e\phi(\mathbf{x})) = e^2 n^2 K \phi(\mathbf{x}),$$

as if $(-e\phi(\mathbf{x}))$ acts like a chemical potential shift, we do find the Thomas-Fermi screening length.

$$-\left(\frac{e}{\omega}\right)^2 \frac{\omega}{2} |E_{||ext}(\mathbf{q}, \omega)|^2 \mathcal{I}m \chi_{||}(\mathbf{q}, \omega),$$

where $\chi''_{||}(\mathbf{q}, \omega)$ is the dissipative current-current response function which is equal to minus the imaginary part of the linear response function. On the other hand

$$\begin{aligned} \mathcal{I}m \chi_{||}(\mathbf{q}, \omega) &= \mathcal{I}m \left(-i \frac{\omega}{e^2} \frac{\sigma_{||}(\mathbf{q}, \omega)}{\epsilon_{||}(\mathbf{q}, \omega)} \right) \\ &= -\frac{\omega}{e^2} \mathcal{R}e \frac{\sigma_{||}(\mathbf{q}, \omega)}{\epsilon_{||}(\mathbf{q}, \omega)} = -\frac{\omega}{e^2} \mathcal{R}e \left(\frac{\omega}{4\pi i} (\epsilon_{||}(\mathbf{q}, \omega) - 1) \frac{1}{\epsilon_{||}(\mathbf{q}, \omega)} \right) \\ &= \frac{\omega^2}{4\pi e^2} \mathcal{I}m \frac{1}{\epsilon_{||}(\mathbf{q}, \omega)}, \\ \mathcal{I}m \chi_{||}(\mathbf{q}, \omega) &= -\frac{\omega}{e^2} \mathcal{R}e \frac{\sigma_{||}(\mathbf{q}, \omega)}{\epsilon_{||}(\mathbf{q}, \omega)} \\ &= -\frac{\omega}{e^2} \mathcal{R}e \left(\frac{\sigma_{||}(\mathbf{q}, \omega)}{1 + \frac{4\pi i}{\omega} \sigma_{||}(\mathbf{q}, \omega)} \right) = -\frac{\omega}{e^2} \frac{1}{|\epsilon_{||}(\mathbf{q}, \omega)|^2} \mathcal{R}e \sigma_{||}(\mathbf{q}, \omega), \end{aligned}$$

which, through $|E_{||ext}| = |\epsilon_{||}| |E_{||int}|$, implies that

$$W = -\frac{\omega}{8\pi} \mathcal{I}m \frac{1}{\epsilon_{||}(\mathbf{q}, \omega)} |E_{||ext}(\mathbf{q}, \omega)|^2 = \frac{1}{2} \mathcal{R}e \sigma_{||}(\mathbf{q}, \omega) |E_{||int}(\mathbf{q}, \omega)|^2. \quad (4.158)$$

Therefore the power dissipation in the presence of a longitudinal field is controlled either by the imaginary part of the inverse dielectric constant or by the real part of the conductivity, depending whether one has access to the applied field or to the full internal one.

In the case of a transverse field

$$W = -\left(\frac{e}{c}\right)^2 \frac{\omega}{2} |A_{\perp int}(\mathbf{q}, \omega)|^2 \mathcal{I}m \widetilde{\chi}_{\perp}(\mathbf{q}, \omega),$$

where

$$\mathcal{I}m \widetilde{\chi}_{\perp}(\mathbf{q}, \omega) = -\frac{\omega}{e^2} \mathcal{R}e \sigma_{\perp}(\mathbf{q}, \omega) = -\frac{\omega^2}{4\pi e^2} \mathcal{I}m \epsilon_{\perp}(\mathbf{q}, \omega).$$

Therefore

$$\begin{aligned} W &= \frac{\omega^2}{2c^2} \mathcal{R}e \sigma_{\perp}(\mathbf{q}, \omega) |A_{\perp int}(\mathbf{q}, \omega)|^2 = \frac{1}{2} \mathcal{R}e \sigma_{\perp}(\mathbf{q}, \omega) |E_{\perp int}(\mathbf{q}, \omega)|^2 \\ &= \frac{\omega}{8\pi} \frac{\omega^2}{c^2} \mathcal{I}m \epsilon_{\perp}(\mathbf{q}, \omega) |A_{\perp int}(\mathbf{q}, \omega)|^2 = \frac{\omega}{8\pi} \mathcal{I}m \epsilon_{\perp}(\mathbf{q}, \omega) |E_{\perp int}(\mathbf{q}, \omega)|^2. \quad (4.159) \end{aligned}$$

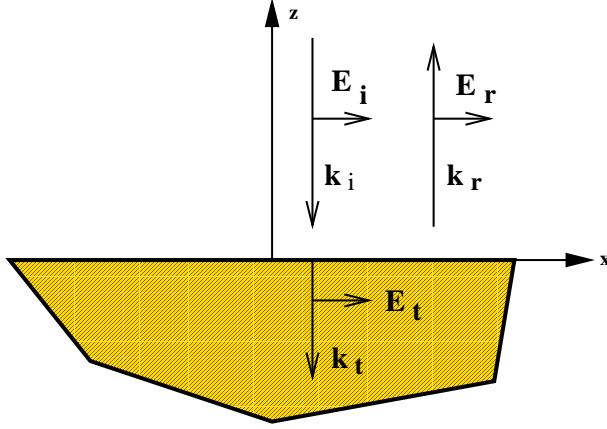


Figure 4.2: Experimental geometry.

4.6.5 Reflectivity

Let us suppose to shoot a beam of light normally to the surface of the sample, which is in contact with the vacuum. The experimental geometry is drawn in Fig. 4.2. The normal direction is the z -direction, so that $z > 0$ is the vacuum and $z < 0$ the sample, and the electric field is polarized along the x -direction. By the geometry of the scattering experiment, the incident, reflected and transmitted waves have all the wave-vector along z , k_i , k_r and k_t , respectively.

Through Eq. (4.136) it derives that the electromagnetic field propagates inside the sample if

$$q^2 = \left(\frac{\omega}{c}\right)^2 \epsilon_{\perp}(\mathbf{q}, \omega).$$

Since the vacuum has $\epsilon_{\perp} = 1$, the conservation of frequency implies

$$k_i^2 = k_r^2 = \frac{k_t^2}{\epsilon_{\perp}(k_t, \omega)},$$

hence $k_r = -k_i > 0$. If the sample is non-magnetic, the electric and magnetic fields, which are both parallel to the surface, should be continuous through the interface vacuum-sample:

$$E_i^x + E_r^x = E_t^x, \quad B_i^y + B_r^y = B_t^y.$$

Notice that

$$B_i^y = \frac{c}{\omega} k_i E_i^x,$$

and analogously for the reflected and transmitted components. Hence $B_i^y + B_r^y = B_t^y$ implies, through $E_i^x + E_r^x = E_t^x$, that

$$k_r (E_r^x - E_i^x) = k_t E_t^x = -\sqrt{\epsilon_{\perp}(k_t, \omega)} k_r (E_i^x + E_r^x),$$

which leads to

$$E_r^x = \frac{1 - \sqrt{\epsilon_{\perp}(k_t, \omega)}}{1 + \sqrt{\epsilon_{\perp}(k_t, \omega)}} E_i^x.$$

Therefore the reflection coefficient is

$$R = \left| \frac{E_r}{E_i} \right|^2 = \left| \frac{1 - \sqrt{\epsilon_{\perp}(k_t, \omega)}}{1 + \sqrt{\epsilon_{\perp}(k_t, \omega)}} \right|^2. \quad (4.160)$$

Since the propagating wave-vector of the light is negligible at the typical excitation frequencies of the sample, we can approximate $\epsilon_{\perp}(k_t, \omega) \simeq \epsilon_{\perp}(0, \omega)$. In a metal we showed that

$$\epsilon_{\perp}(\mathbf{0}, \omega) = 1 - \frac{\omega_p^2}{\omega^2},$$

which is real and negative for $|\omega| < \omega_p$. Through Eq. (4.160) it implies that a metal reflects perfectly for frequencies below the plasma frequency.

4.7 Random Phase Approximation for the electron gas

So far we have introduced the linear response functions of an electron gas and discussed some limiting values which can be obtained without resorting to any explicit calculation. In this section we will evaluate the response functions within the time-dependent Hartree-Fock approximation.

As before we consider an electron gas in the presence of a positive background which neutralizes its charge. The Hamiltonian is

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \frac{1}{2V} \sum_{\mathbf{k}\mathbf{p}\mathbf{q}} U(\mathbf{q}) (\rho(\mathbf{q}) - V n_{\mathbf{q}\mathbf{0}}) (\rho(-\mathbf{q}) - V n_{-\mathbf{q}\mathbf{0}}), \quad (4.161)$$

where $\epsilon_{\mathbf{k}} = \hbar^2 |\mathbf{k}|^2 / 2m$ is the kinetic energy, $U(\mathbf{q}) = 4\pi e^2 / |\mathbf{q}|^2$ and $\rho(\mathbf{q})$ the Fourier transforms of the Coulomb interaction and of the electron density, respectively, and n the positive background density. By definition the Fourier transform of the electron density at $\mathbf{q} = \mathbf{0}$ is equal to $V n$, thus canceling the positive background charge. Therefore the interaction term is actually

$$\mathcal{H}_{int} = \frac{1}{V} \sum_{\mathbf{q} \neq \mathbf{0}} \sum_{\mathbf{k}\mathbf{p}} U(\mathbf{q}) \rho(\mathbf{q}) \rho(-\mathbf{q}). \quad (4.162)$$

Let us start with the Hartree-Fock approximation. If we assume that spin-rotational and space-translational symmetries are preserved in the actual ground state, then we are forced to search for an Hartree-Fock wave-function whose only variational parameters are

$$\langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \rangle = n_{\mathbf{k}\sigma}, \quad (4.163)$$

with $n_{\mathbf{k}\uparrow} = n_{\mathbf{k}\downarrow} = n_{\mathbf{k}}$. Then, for $\mathbf{q} \neq \mathbf{0}$,

$$\begin{aligned} \rho(\mathbf{q}) \rho(-\mathbf{q}) &= \sum_{\mathbf{k}\mathbf{p}} \sum_{\sigma\sigma'} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{p}+\mathbf{q}\sigma'}^\dagger c_{\mathbf{p}\sigma'} \\ &\rightarrow - \sum_{\mathbf{k}\sigma} n_{\mathbf{k}} c_{\mathbf{k}+\mathbf{q}\sigma}^\dagger c_{\mathbf{k}+\mathbf{q}\sigma} + n_{\mathbf{k}+\mathbf{q}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}, \end{aligned}$$

so that the Hartree-Fock Hamiltonian is

$$\mathcal{H}_{HF} = \sum_{\mathbf{k}\sigma} \left(\epsilon_{\mathbf{k}} - \frac{1}{V} \sum_{\mathbf{q} \neq \mathbf{0}} U(\mathbf{q}) n_{\mathbf{k}+\mathbf{q}} \right) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}, \quad (4.164)$$

which is already diagonal with eigenvalues

$$\epsilon_{\mathbf{k}HF} = \epsilon_{\mathbf{k}} - \frac{1}{V} \sum_{\mathbf{q} \neq \mathbf{0}} U(\mathbf{q}) n_{\mathbf{k}+\mathbf{q}}.$$

Let us assume that the Fermi-sea solution, i.e. $n_{\mathbf{k}} = 1$ if $|\mathbf{k}| < k_F$ and zero otherwise, is still the choice which minimizes the total energy, and let us apply the time-dependent Hartree-Fock machinery to evaluate the response to an external field $V_{ext}(\mathbf{q}, t)$ which couples to the density. We readily find that the equation of motion of the average values

$$\Delta_{\mathbf{k}, \mathbf{k}+\mathbf{q}; \sigma} = \langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}+\mathbf{q}\sigma} \rangle,$$

is, at linear order,

$$(i\hbar\partial_t - \epsilon_{\mathbf{k}+\mathbf{q}HF} + \epsilon_{\mathbf{k}HF}) \Delta_{\mathbf{k}, \mathbf{k}+\mathbf{q}; \sigma} = (n_{\mathbf{k}} - n_{\mathbf{k}+\mathbf{q}}) \left[V_{ext}(\mathbf{q}, t) + \frac{1}{V} \sum_{\mathbf{p}\sigma'} \Delta_{\mathbf{p}, \mathbf{p}+\mathbf{q}; \sigma'} (U(\mathbf{q}) - \delta_{\sigma\sigma'} U(\mathbf{k} - \mathbf{p})) \right].$$

Let us solve this equation neglecting the second term, i.e. the Fock contribution, in the right hand side, which corresponds to the so-called Random Phase Approximation (RPA). To be consistent, the RPA approximation also amounts to neglect the interaction correction to the HF eigenvalues, which only derives from the Fock term, so that $\epsilon_{\mathbf{k}HF} \rightarrow \epsilon_{\mathbf{k}}$. Within RPA we find that

$$\Delta_{\mathbf{k}, \mathbf{k}+\mathbf{q}; \sigma} = \frac{n_{\mathbf{k}} - n_{\mathbf{k}+\mathbf{q}}}{\omega - \epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}}} \left[V_{ext}(\mathbf{q}, t) + \frac{U(\mathbf{q})}{V} \sum_{\mathbf{p}\sigma'} \Delta_{\mathbf{p}, \mathbf{p}+\mathbf{q}; \sigma'} \right]. \quad (4.165)$$

The induced charge is defined for as

$$\rho_{ind}(\mathbf{q}, \omega) = \sum_{\mathbf{k}\sigma} \langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}+\mathbf{q}\sigma} \rangle - V n \delta_{\mathbf{q}0},$$

and satisfy the RPA equation

$$\begin{aligned} \rho_{ind}(\mathbf{q}, \omega) &= \left(\sum_{\mathbf{k}\sigma} \frac{n_{\mathbf{k}} - n_{\mathbf{k}+\mathbf{q}}}{\omega - \epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}}} \right) \left[V_{ext}(\mathbf{q}, t) + \frac{U(\mathbf{q})}{V} \sum_{\mathbf{p}\sigma'} \Delta_{\mathbf{p}, \mathbf{p}+\mathbf{q}; \sigma'} \right] \\ &\equiv V \tilde{\chi}_{RPA}(\mathbf{q}, \omega) \left[V_{ext}(\mathbf{q}, t) + \frac{U(\mathbf{q})}{V} \rho_{ind}(\mathbf{q}, \omega) \right], \end{aligned}$$

where

$$\tilde{\chi}_{RPA}(\mathbf{q}, \omega) = \frac{1}{V} \sum_{\mathbf{k}\sigma} \frac{n_{\mathbf{k}} - n_{\mathbf{k}+\mathbf{q}}}{\omega - \epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}} + i\eta} \quad (4.166)$$

corresponds to the proper density-density response function within RPA, the infinitesimal $\eta > 0$ playing the role of the adiabatic switching rate.

$\tilde{\chi}_{RPA}(\mathbf{q}, \omega)$ is also the density-density response function of free electrons, also called the Lindhart function, which also clarifies the meaning of the RPA approximation. As we know the

proper response function is the response to the external field plus the electric field generated by the same electrons. In order not to double-count this term, the proper response function has to be evaluated neglecting the contribution of the electron-electron Coulomb repulsion which represents the coupling of the electrons to the average electric field generated by the same electrons, which is roughly as if the electrons were actually non-interacting. We leave as an exercise the evaluation of the Lindhart function in a three-dimensional. We just mention that the RPA approximation preserves the sum-rule (4.140), hence all the results which derives from that. Concerning the limiting value (4.152), within RPA the compressibility turns out to be that one for free electrons.

One can perform the same analysis with an external probe which couples to the transverse current. The result would be a transverse current-current response function which, within the RPA approximation, coincides with that of free electrons. Also in this case the exact limiting values we have previously extracted are reproduced. In other words the Random Phase is a consistent Approximation.

Excercises

- (3) Calculate the Lindhart function for an $\epsilon_{\mathbf{k}} = \hbar^2 k^2 / 2m$ dispersion in three dimensions.
- (4) Calculate the

$$\lim_{\mathbf{q} \rightarrow \mathbf{0}} \lim_{\omega \rightarrow 0} \tilde{\chi}_{\perp}(\mathbf{q}, \omega),$$

of the transverse current-current response function for free electrons. Show that the limit coincides with (4.156) with $A = 4$. Prove that the diamagnetic term is actually $1/3$ of the paramagnetic one.

Chapter 5

Feynamm diagram technique

Time-dependent Hartree-Fock is a relatively simple way to access excitation properties thus going beyond Hartree-Fock theory. A more systematic scheme, which includes time-dependent Hartree-Fock as an approximation, is to perform perturbation theory. However the perturbation expansion in a many-body problem is not as straightforward as in a single-body case but can be simplified substantially by means of the so-called Feynamm diagram technique. In this chapter we present this technique at finite temperature.

5.1 Preliminaries

First of all we need some preliminary definitions and results.

5.1.1 Imaginary-time ordered products

Let us introduce first the imaginary time evolution of an operator $A(\mathbf{x})$ through

$$A(\mathbf{x}, \tau) = e^{H\tau} A(\mathbf{x}) e^{-H\tau}, \quad (5.1)$$

where H is the fully interacting Hamiltonian and $\tau \in [0, \beta]$, where $\beta = 1/T$ is the inverse temperature (we use $\hbar = 1$ and $K_B = 1$).

Given two operators $A(\mathbf{x})$ and $B(\mathbf{y})$ we define the imaginary time Green's function through

$$\begin{aligned} G_{AB}(\mathbf{x}, \mathbf{y}; \tau - \tau') &= -\langle T_\tau (A(\mathbf{x}, \tau) B(\mathbf{y}, \tau')) \rangle \\ &= -\theta(\tau - \tau') \langle A(\mathbf{x}, \tau) B(\mathbf{y}, \tau') \rangle + \theta(\tau' - \tau) \langle B(\mathbf{y}, \tau') A(\mathbf{x}, \tau) \rangle. \end{aligned} \quad (5.2)$$

where T_τ denotes the time-ordered product, and the minus sign applies when one or both the operators are bosonic-like, namely contain bosons or an even product of fermionic operators, while the plus sign when both operators are fermionic-like, i.e. contain an odd product of

fermionic operators. Due to time-translation invariance, the Green's functions only depend on the time difference $\tau - \tau' \in [-\beta, \beta]$.

Analogously, given n operators, $A_i(\mathbf{x}_i, \tau_i)$, $i = 1, \dots, n$, we can define the multi-operator Green's function

$$G_{A_1, \dots, A_n}(\mathbf{x}_1, \dots, \mathbf{x}_n; \tau_1, \dots, \tau_n) = -\langle T_\tau (A_1(\mathbf{x}_1, \tau_1) \dots A_n(\mathbf{x}_n, \tau_n)) \rangle, \quad (5.3)$$

which is the average of the time ordered product, namely operators with earlier times appear on the right of those at later times, having a minus sign if the number of crossings needed to bring fermionic-like operators in the correct time-ordered sequence is even and the sign plus otherwise.

5.1.2 Matsubara frequencies

Let us consider the two-operator Green's function $G_{AB}(\mathbf{x}, \mathbf{y}; \tau)$, with $\tau \in [-\beta, \beta]$ being the time difference. Since the time domain is bounded, we can introduce a discrete Fourier transform, with frequencies $\omega_n = (2\pi/2\beta)n = \pi n T$, with n an integer. We define, dropping for simplicity the spatial dependence,

$$G_{AB}(i\omega_n) = \frac{1}{2} \int_{-\beta}^{\beta} d\tau e^{i\omega_n \tau} G_{AB}(\tau),$$

and, consequently,

$$G_{AB}(\tau) = T \sum_n e^{-i\omega_n \tau} G_{AB}(i\omega_n).$$

From the properties of the trace it derives that

$$\begin{aligned} \langle B(0) A(\tau) \rangle &= \frac{1}{Z} \text{Tr} \left[e^{-\beta H} B e^{H\tau} A e^{H-\tau} \right] \\ &= \frac{1}{Z} \text{Tr} \left[e^{-\beta H} e^{\beta H} e^{H\tau} A e^{-H\tau} e^{-\beta H} B \right] = \langle A(\beta + \tau) B(0) \rangle, \end{aligned}$$

which implies that

$$\begin{aligned} G_{AB}(i\omega_n) &= \frac{1}{2} \int_{-\beta}^{\beta} d\tau e^{i\omega_n \tau} G_{AB}(\tau) \\ &= -\frac{1}{2} \int_0^\beta d\tau e^{i\omega_n \tau} \langle A(\tau) B(0) \rangle \mp \frac{1}{2} \int_{-\beta}^0 d\tau e^{i\omega_n \tau} \langle B(0) A(\tau) \rangle \\ &= -\frac{1}{2} \int_0^\beta d\tau e^{i\omega_n \tau} \langle A(\tau) B(0) \rangle \mp \frac{1}{2} \int_{-\beta}^0 d\tau e^{i\omega_n \tau} \langle A(\beta + \tau) B(0) \rangle \\ &= -\frac{1}{2} \int_0^\beta d\tau e^{i\omega_n \tau} \langle A(\tau) B(0) \rangle \mp \frac{1}{2} e^{-i\omega_n \beta} \int_0^\beta d\tau e^{i\omega_n \tau} \langle A(\tau) B(0) \rangle \\ &= \frac{1}{2} (1 \pm e^{-i\omega_n \beta}) \int_0^\beta d\tau e^{i\omega_n \tau} G_{AB}(\tau). \end{aligned}$$

Since $\exp(-i\omega_n\beta) = (-1)^n$ then a non-zero Fourier transform requires for bosonic-like operators even integers n 's and for fermionic-like odd n 's. We define the bosonic Matsubara frequencies

$$\Omega_m = 2m\pi T \quad (5.4)$$

and the fermionic Matsubara frequencies

$$\omega_m = (2m+1)\pi T, \quad (5.5)$$

so that the bosonic- and fermionic-like Fourier transform of $G_{AB}(\tau)$ become, respectively,

$$G_{AB}(\Omega_m) = \int_0^\beta d\tau e^{i\Omega_m\tau} G_{AB}(\tau), \quad G_{AB}(\omega_m) = \int_0^\beta d\tau e^{i\omega_m\tau} G_{AB}(\tau), \quad (5.6)$$

hence just require the knowledge of the Green's functions for positive τ .

Connection between bosonic Green's functions and linear response functions

Let us assume that both A and B are observable quantities, which implies they are hermitean, hence bosonic-like operators. Then, for positive τ , we have

$$\begin{aligned} G_{AB}(\tau) &= -\langle A(\tau)B(0) \rangle = -\frac{1}{Z} \sum_n e^{-\beta E_n} \langle n | e^{H\tau} A e^{-H\tau} B | n \rangle \\ &= -\frac{1}{Z} \sum_{nm} e^{-\beta E_n} e^{-(E_m-E_n)\tau} \langle n | A | m \rangle \langle m | B | n \rangle. \end{aligned}$$

Since

$$\int_0^\beta d\tau e^{i\Omega_l\tau} e^{-(E_m-E_n)\tau} = \frac{1}{i\Omega_l - (E_m - E_n)} \left(e^{-(E_m - E_n)\beta} - 1 \right),$$

we finally find that

$$G_{AB}(i\Omega_l) = \frac{1}{Z} \sum_{nm} \left(e^{-\beta E_n} - e^{-\beta E_m} \right) \frac{1}{i\Omega_l - (E_m - E_n)} \langle n | A | m \rangle \langle m | B | n \rangle. \quad (5.7)$$

Comparing this expression with the Fourier transform in frequency of the linear response function $\chi_{AB}(\omega)$, see Eq. (3.33), we easily realize that the two coincide if we analytically continue $G_{AB}(i\Omega_l)$ on the real axis, $i\Omega_l \rightarrow \omega + i\eta$. In other words the knowledge of $G_{AB}(i\Omega_l)$ means that we know the value of the function $G_{AB}(z)$ of the complex variable z on an infinite set of points on the imaginary axis $z_l = i\Omega_l$. This is sufficient to determine the full $G_{AB}(z)$ in the complex plane, with the supplementary condition that, since $G_{AB}(z) = \chi_{AB}(z)$, it has to be analytic in the upper half-plane.

Useful formulas

There is a very useful trick to perform summation over Matsubara frequencies. Let us start from the fermionic case. Suppose we have to calculate

$$T \sum_n F(i\epsilon_n),$$

where we assume that $F(z)$ vanishes faster than $1/|z|$ for $|z| \rightarrow \infty$ and has poles but on the imaginary axis. We notice that the Fermi distribution function, as function of a complex variable,

$$f(z) = \frac{1}{e^{\beta z} + 1},$$

has poles at

$$z_n = i(2n+1)\frac{\pi}{\beta} = i\epsilon_n,$$

namely right at the Matsubara frequencies, with residue $-T$. Let us consider the integral along the contour shown in Fig. 5.1

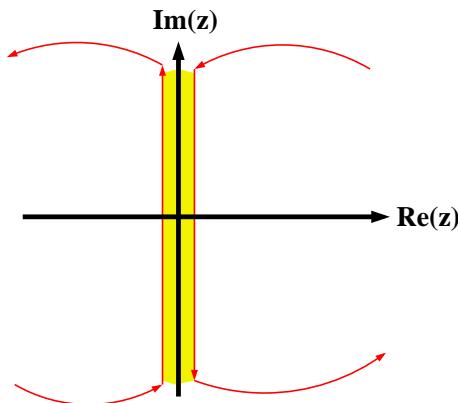


Figure 5.1: Integration countour, see text.

$$I = \oint \frac{dz}{2\pi i} f(z) F(z).$$

This countour integral can be calculated by catching all poles of the integrand in the region enclosed by the countour which includes the imaginary axis, shaded area in Fig. 5.1. Since this area is enclosed clockwise the integral gives

$$I = - \sum_{z_n} \text{Res}(f(z_n)) F(z_n) = T \sum_n F(i\epsilon_n),$$

which is just the sum we want to calculate. On the other hand, I can be equally calculated by catching all poles of the integrand in the area which does not include the imaginary axis, the non-shaded region, which, being enclosed anti-clockwise gives

$$I = \sum_{z_* = \text{poles of } F(z)} f(z_*) \operatorname{Res}(F(z_*)).$$

Therefore

$$T \sum_n F(i\epsilon_n) = \sum_{z_* = \text{poles of } F(z)} f(z_*) \operatorname{Res}(F(z_*)). \quad (5.8)$$

Notice that, if $F(z)$ has branch cuts the calculation is slightly more complicated since we have to deform the contour as to avoid branch cuts. In this case, instead of catching poles we have to integrate along branch cuts. For instance, suppose that $F(z)$ has a branch cut at $z = x + i\omega$, with $x \in [-\infty, \infty]$, as shown in Fig. 5.2. Let us consider the non-shaded area enclosed inside

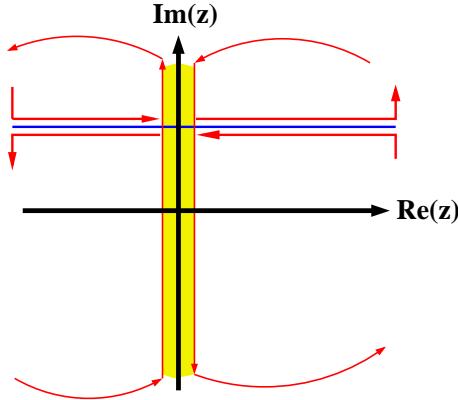


Figure 5.2: Integration countour in the presence of a branch cut, see text.

the countour depicted in Fig. 5.2. In this area there are no poles hence the contour integral is zero. On the other hand this contour integral is also equal to the contribution of the poles inside the shaded area, which includes the imaginary axis, plus the integral along the contour which encloses the branch cut. Therefore

$$T \sum_n F(i\epsilon_n) = - \int \frac{dx}{2\pi i} f(x + i\omega) [F(x + i\omega + i0^+) - F(x + i\omega - i0^+)]. \quad (5.9)$$

In the case in which the summation is performed over bosonic frequencies, we can use similar tricks once we recognize that the poles of the Bose distribution function

$$b(z) = \frac{1}{e^{\beta z} - 1},$$

coincide with the bosonic Matsubara frequencies,

$$z_n = i 2n \frac{\pi}{\beta},$$

with residue T .

5.1.3 Single-particle Green's functions

Among the averages of time-ordered products an important role in the diagrammatic technique is played by the so-called single-particle Green's functions.

Fermionic case

If $\Psi_\sigma(\mathbf{x}, \tau)$ is the imaginary-time evolution of the Fermi field, then the single-particle Green's functions is defined through

$$\begin{aligned} G_{\sigma\sigma'}(\mathbf{x}, \mathbf{y}; \tau) &= -\langle T_\tau (\Psi_\sigma(\mathbf{x}, \tau) \ \Psi_{\sigma'}(\mathbf{y})^\dagger) \rangle \\ &= -\theta(\tau) \langle \Psi_\sigma(\mathbf{x}, \tau) \ \Psi_{\sigma'}(\mathbf{y})^\dagger \rangle + \theta(-\tau) \langle \Psi_{\sigma'}(\mathbf{y})^\dagger \Psi_\sigma(\mathbf{x}, \tau) \rangle. \end{aligned} \quad (5.10)$$

If we make a spectral representation as before and calculate the Fourier transform using the fermionic Matsubara frequency, we readily find that

$$G_{\sigma\sigma'}(\mathbf{x}, \mathbf{y}; i\omega_l) = \frac{1}{Z} \sum_{nm} \left(e^{-\beta E_n} + e^{-\beta E_m} \right) \frac{1}{i\Omega_l - (E_m - E_n)} \langle n | \Psi_\sigma(\mathbf{x}) | m \rangle \langle m | \Psi_{\sigma'}(\mathbf{y})^\dagger | n \rangle.$$

Let us take $\sigma = \sigma'$ and $\mathbf{x} = \mathbf{y}$, which correspond to the so-called local Green's function, and introduce the real and positive spectral function

$$A_\sigma(\mathbf{x}, \epsilon) = \frac{1}{Z} \sum_{nm} \left(e^{-\beta E_n} + e^{-\beta E_m} \right) \left| \langle n | \Psi_\sigma(\mathbf{x}) | m \rangle \right|^2 \delta(\epsilon - E_m + E_n),$$

through which, after continuation in the complex plane $i\omega_l \rightarrow z$

$$G_{\sigma\sigma}(\mathbf{x}, \mathbf{x}; z) = \int d\epsilon A_\sigma(\mathbf{x}, \epsilon) \frac{1}{z - \epsilon}.$$

As function of the complex frequency, $G(z)$ has generally branch cut singularities along the real axis. Indeed

$$G_{\sigma\sigma}(\mathbf{x}, \mathbf{x}; z = \omega + i0^+) - G_{\sigma\sigma}(\mathbf{x}, \mathbf{x}; z = \omega - i0^+) = -2\pi i A_\sigma(\mathbf{x}, \omega).$$

What is the physical meaning of the spectral function? Let us rewrite $A_\sigma(\mathbf{x}, \omega)$ in the following equivalent way:

$$\begin{aligned} A_\sigma(\mathbf{x}, \epsilon) &= \sum_{nm} \frac{e^{-\beta E_n}}{Z} \left| \langle m | \Psi_\sigma(\mathbf{x})^\dagger | n \rangle \right|^2 \delta(\epsilon - E_m + E_n) \\ &\quad + \sum_{nm} \frac{e^{-\beta E_n}}{Z} \left| \langle m | \Psi_\sigma(\mathbf{x}) | n \rangle \right|^2 \delta(\epsilon + E_m - E_n), \end{aligned} \quad (5.11)$$

which shows more explicitly that $A_\sigma(\mathbf{x}, \omega)$ is just the local density of states for adding, first term in the right hand side, or removing, second term, a particle at position \mathbf{x} with spin σ . This quantity can be for instance measured in tunneling experiments. Finally we notice that

$$\begin{aligned} \int d\epsilon A_\sigma(\mathbf{x}, \epsilon) &= \sum_{nm} \frac{e^{-\beta E_n}}{Z} \left(\left| \langle m | \Psi_\sigma(\mathbf{x})^\dagger | n \rangle \right|^2 + \left| \langle m | \Psi_\sigma(\mathbf{x}) | n \rangle \right|^2 \right) \\ &= \sum_n \frac{e^{-\beta E_n}}{Z} (\langle n | \Psi_\sigma(\mathbf{x}) \Psi_\sigma(\mathbf{x})^\dagger | n \rangle + \langle n | \Psi_\sigma(\mathbf{x})^\dagger \Psi_\sigma(\mathbf{x}) | n \rangle) \\ &= \sum_n \frac{e^{-\beta E_n}}{Z} \langle n | \{ \Psi_\sigma(\mathbf{x}), \Psi_\sigma(\mathbf{x})^\dagger \} | n \rangle = 1, \end{aligned}$$

namely that the integral of the spectral function is normalized to one.

In all this chapter we are going to assume a grand-canonical ensamble for the fermions, which is equivalent to add to the fermionic Hamiltonian H a chemical potential term, i.e. $H \rightarrow H - \mu N$, where μ is such that the average number of particles has the desired value N_0 . At $T = 0$ μ becomes the Fermi energy and selects as the ground state the lowest energy state with N_0 particles. Therefore, at $T = 0$ the sum over n is reduced just to the ground state, $|0, N_0\rangle$, with N_0 particles, hence

$$\begin{aligned} A_\sigma(\mathbf{x}, \epsilon) &= \sum_m \delta(\epsilon + E_0(N_0) - E_m(N_0 + 1)) \left| \langle m, N_0 + 1 | \Psi_\sigma(\mathbf{x})^\dagger | 0, N_0 \rangle \right|^2 \\ &\quad + \sum_m \delta(\epsilon - E_0(N_0) + E_m(N_0 - 1)) \left| \langle m, N_0 - 1 | \Psi_\sigma(\mathbf{x}) | 0, N_0 \rangle \right|^2, \end{aligned}$$

where we explicitly indicate that the ground state energy refers to N_0 particles and the first term in the right hand side involves moving to the subspace with $N_0 + 1$ electrons, and the second to the subspace with $N_0 - 1$ electrons. The first δ -function implies that

$$\epsilon = E_m(N_0 + 1) - E_0(N_0) = (E_m(N_0 + 1) - E_0(N_0 + 1)) + (E_0(N_0 + 1) - E_0(N_0)) \geq 0,$$

because the energy of the state m with $N_0 + 1$ electrons is greater or equal to the ground state energy $E_0(N_0 + 1)$, and, by definition, $E_0(N_0 + 1) - E_0(N_0) \geq 0$ since the lowest energy state for any N occurs at N_0 . Analogously, in the second δ -function

$$\epsilon = -(E_0(N_0 - 1) - E_0(N_0)) - (E_m(N_0 - 1) - E_0(N_0 - 1)) \leq 0.$$

In other words, for positive ϵ the spectral function is the density of states upon adding an electron and for negative values that one for removing one particle.

Let us suppose now that the system is translationally invariant. If we then expand the Fermi fields in eigenstates of the crystalline momentum, and introduce the space Fourier transform of the Green's function, we find

$$G_{\sigma\sigma'}(\mathbf{k}, \mathbf{p}; \tau) = -\langle T_\tau \left(c_{\mathbf{k}\sigma}(\tau) c_{\mathbf{p}\sigma'}^\dagger \right) \rangle = \delta_{\mathbf{k}\mathbf{p}} G_{\sigma\sigma'}(\mathbf{k}, \tau),$$

where

$$G_{\sigma\sigma'}(\mathbf{k}, \tau) = -\langle T_\tau \left(c_{\mathbf{k}\sigma}(\tau) c_{\mathbf{k}\sigma'}^\dagger \right) \rangle. \quad (5.12)$$

In this case and for $\sigma = \sigma'$ the Fourier transform in the complex frequency plane would be

$$G_{\sigma\sigma}(\mathbf{k}, z) = \int d\epsilon A_\sigma(\mathbf{k}, \epsilon) \frac{1}{z - \epsilon},$$

where

$$A_\sigma(\mathbf{k}, \epsilon) = \frac{1}{Z} \sum_{nm} \left(e^{-\beta E_n} + e^{-\beta E_m} \right) \left| \langle n | c_{\mathbf{k}\sigma} | m \rangle \right|^2 \delta(\epsilon - E_m + E_n), \quad (5.13)$$

is the density of states for adding and removing a particle at momentum \mathbf{k} . Since $A(\mathbf{k}, \epsilon)$ is real and positive, $G(\mathbf{k}, z)$ has generally branch cuts on the real axis, since

$$G_{\sigma\sigma}(\mathbf{k}, \epsilon + i0^+) - G_{\sigma\sigma}(\mathbf{k}, \epsilon - i0^+) = -2\pi i A_\sigma(\mathbf{k}, \epsilon). \quad (5.14)$$

Notice that, as before, the spectral function is normalized to one. In addition one can readily verify that

$$A_\sigma(\mathbf{x}, \epsilon) = A_\sigma(\epsilon) = \frac{1}{V} \sum_{\mathbf{k}} A_\sigma(\mathbf{k}, \epsilon). \quad (5.15)$$

Let us consider non-interacting electrons described by the Hamiltonian

$$H_0 = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma},$$

where, as discussed previously, $\epsilon_{\mathbf{k}}$ is measured with respect to the chemical potential μ , which is the Fermi energy at $T = 0$. In this case it is easy to show that

$$G_{\sigma\sigma'}^{(0)}(\mathbf{k}, i\omega_n) = \delta_{\sigma\sigma'} G^{(0)}(\mathbf{k}, i\omega_n),$$

where

$$G^{(0)}(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n - \epsilon_{\mathbf{k}}}. \quad (5.16)$$

The spectral function is simply

$$A^{(0)}(\mathbf{k}, \epsilon) = \delta(\epsilon - \epsilon_{\mathbf{k}}), \quad (5.17)$$

and is finite for $\epsilon > 0$ if \mathbf{k} is outside the Fermi surface, and for $\epsilon < 0$ otherwise. Notice that a small frequency ϵ corresponds to small $\epsilon_{\mathbf{k}}$, i.e. to momenta close to the Fermi surface.

Bosonic case

Let us define as $\Phi(\mathbf{x})$ the Bose field for spinless bosons. Analogously to the fermionic case we can define a single-particle Green's function through

$$\begin{aligned} G(\mathbf{x}, \mathbf{y}; \tau) &= -\langle T_{\tau} (\Phi(\mathbf{x}, \tau) \Phi(\mathbf{y})^{\dagger}) \rangle \\ &= -\theta(\tau) \langle \Phi(\mathbf{x}, \tau) \Phi(\mathbf{y})^{\dagger} \rangle - \theta(-\tau) \langle \Phi(\mathbf{y})^{\dagger} \Phi(\mathbf{x}, \tau) \rangle. \end{aligned}$$

Let us again assume that the model is translationally invariant and introduce the bosonic operators $a_{\mathbf{q}}$ and $a_{\mathbf{q}}^{\dagger}$, as well as the conjugate variables

$$\begin{aligned} x_{\mathbf{q}} &= \sqrt{\frac{1}{2}} (a_{\mathbf{q}} + a_{-\mathbf{q}}^{\dagger}), \\ p_{\mathbf{q}} &= -i \sqrt{\frac{1}{2}} (a_{\mathbf{q}} - a_{-\mathbf{q}}^{\dagger}). \end{aligned}$$

In most common situations, the object which appears within perturbation theory is, rather than the single-particle Green's function, the $x - x$ time-ordered product, namely

$$D(\mathbf{q}, \tau) = -\langle T_{\tau} (x_{\mathbf{q}}(\tau) x_{-\mathbf{q}}) \rangle. \quad (5.18)$$

Let us consider the bosonic non-interacting Hamiltonian

$$H_0 = \sum_{\mathbf{q}} \omega_{\mathbf{q}} a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}},$$

with $\omega_{\mathbf{q}} = \omega_{-\mathbf{q}}$. Then, for positive τ ,

$$\begin{aligned} D(\mathbf{q}, \tau) &= -\frac{1}{2} \langle a_{\mathbf{q}}(\tau) a_{\mathbf{q}}^{\dagger} \rangle - \frac{1}{2} \langle a_{-\mathbf{q}}^{\dagger}(\tau) a_{-\mathbf{q}} \rangle \\ &= -\frac{1}{2} e^{-\omega_{\mathbf{q}} \tau} (1 + b(\omega_{\mathbf{q}})) - \frac{1}{2} e^{\omega_{\mathbf{q}} \tau} b(\omega_{\mathbf{q}}), \end{aligned}$$

where

$$b(\omega_{\mathbf{q}}) = \langle a_{\mathbf{q}}^\dagger a_{\mathbf{q}} \rangle = \left(e^{\omega_{\mathbf{q}} \beta} - 1 \right)^{-1},$$

is the Bose distribution function, and

$$\langle a_{\mathbf{q}} a_{\mathbf{q}}^\dagger \rangle = 1 + b(\omega_{\mathbf{q}}) = - \left(e^{-\omega_{\mathbf{q}} \beta} - 1 \right)^{-1}.$$

Noticing that

$$\int_0^\beta d\tau e^{i\Omega_m \tau} e^{\mp \omega_{\mathbf{q}} \tau} = \frac{1}{i\Omega_m \mp \omega_{\mathbf{q}}} \left(e^{\mp \omega_{\mathbf{q}} \beta} - 1 \right),$$

one readily finds that

$$D^{(0)}(\mathbf{q}, i\Omega_m) = \frac{1}{2} \left(\frac{1}{i\Omega_m - \omega_{\mathbf{q}}} - \frac{1}{i\Omega_m + \omega_{\mathbf{q}}} \right) = - \frac{\omega_{\mathbf{q}}}{\Omega_m^2 + \omega_{\mathbf{q}}^2}. \quad (5.19)$$

5.2 Perturbation expansion in imaginary time

Let us suppose that the full Hamiltonian

$$H = H_0 + V,$$

where H_0 is a single particle Hamiltonian which can be diagonalized exactly while V is a perturbation which makes the model not solvable, e.g. it is the electron-electron interaction. We already showed in Section 4.2 that

$$e^{-\tau H} = e^{-\tau H_0} S(\tau),$$

where, see Eq. (4.28),

$$S(\tau) \equiv S(\tau, 0) = T_\tau \left[\exp \left(- \int_0^\tau d\tau_1 V(\tau_1) \right) \right], \quad (5.20)$$

being $V(\tau)$ the Heisenberg evolution of V with the non-interacting Hamiltonian. It is easy to show that, for $\tau \geq \tau'$,

$$\begin{aligned} S(\tau - \tau', 0) &= T_\tau \left[\exp \left(- \int_0^{\tau - \tau'} d\tau_1 V(\tau_1) \right) \right] = T_\tau \left[\exp \left(- \int_{\tau'}^\tau d\tau_1 V(\tau_1 - \tau') \right) \right] \\ &= e^{-\tau' H_0} T_\tau \left[\exp \left(- \int_{\tau'}^\tau d\tau_1 V(\tau_1) \right) \right] e^{\tau' H_0} \equiv e^{-\tau' H_0} S(\tau, \tau') e^{\tau' H_0}, \end{aligned}$$

namely that

$$e^{-(\tau - \tau') H} = e^{-\tau H_0} S(\tau, \tau') e^{\tau' H_0}. \quad (5.21)$$

Suppose we have to calculate the multi-operator Green's function (5.3), and further assume that, e.g., $\tau_1 \geq \tau_2 \geq \dots \geq \tau_{n-1} \geq \tau_n$, then

$$\begin{aligned} G_{A_1, \dots, A_n}(\tau_1, \dots, \tau_n) &= -\langle A_1(\tau_1) \dots A_n(\tau_n) \rangle \\ &= \frac{1}{Z} \text{Tr} \left[e^{-\beta H} e^{\tau_1 H} A_1 e^{-\tau_1 H} e^{\tau_2 H} A_2 e^{-\tau_2 H} \dots e^{-\tau_{n-1} H} e^{\tau_n H} A_n e^{-\tau_n H} \right] \\ &= \frac{1}{Z} \text{Tr} \left[e^{-\beta H_0} S(\beta, \tau_1) e^{\tau_1 H_0} A_1 e^{-\tau_1 H_0} S(\tau_1, \tau_2) e^{\tau_2 H_0} A_2 e^{-\tau_2 H_0} \dots \right. \\ &\quad \left. \dots S(\tau_{n-1}, \tau_n) e^{\tau_n H_0} A_n e^{-\tau_n H_0} S(\tau_n, 0) \right]. \end{aligned}$$

We readily see that all times remain ordered, so that for a generic time-ordering we would get

$$\begin{aligned} G_{A_1, \dots, A_n}(\tau_1, \dots, \tau_n) &= -\langle T_\tau (A_1(\tau_1) \dots A_n(\tau_n)) \rangle \\ &= \frac{1}{Z} \text{Tr} \left[e^{-\beta H_0} T_\tau (S(\beta) A_1(\tau_1) \dots A_n(\tau_n)) \right], \end{aligned}$$

where the time evolution of the A_i 's operators in the last equation is through the non-interacting Hamiltonian. Recalling that

$$Z = Z_0 \langle S(\beta) \rangle,$$

we therefore conclude that

$$G_{A_1, \dots, A_n}(\tau_1, \dots, \tau_n) = -\frac{1}{\langle S(\beta) \rangle} \langle T_\tau (S(\beta) A_1(\tau_1) \dots A_n(\tau_n)) \rangle, \quad (5.22)$$

where the thermal averages as well as the imaginary-time evolution are done with the non-interacting Hamiltonian H_0 . This expression is now suitable for an expansion in V .

5.2.1 Wick's theorem

Upon expanding $S(\beta)$ in powers of the perturbation V , the calculation of any Green's function reduces to evaluate the average value of a time-ordered product of Fermi or Bose fields with a non interacting Hamiltonian. It is therefore essential to know how to perform this calculation.

Let us suppose to evaluate with a non-interacting Hamiltonian for free fermions the average value

$$-\langle T_\tau \left(\Psi(\mathbf{x}_1, \tau_1) \Psi(\mathbf{x}_2, \tau_2) \dots \Psi(\mathbf{x}_n, \tau_n) \Psi(\mathbf{y}_n, \tau'_n)^\dagger \dots \Psi(\mathbf{y}_1, \tau'_1)^\dagger \right) \rangle.$$

For any time-ordering this amounts to average a product of creation and annihilation operators over a non interacting Hamiltonian. We already know that this is the sum of the products of all possible contractions of an annihilation with a creation operator. Suppose that the operator $\Psi(\mathbf{x}_i, \tau_i)$ is contracted with $\Psi(\mathbf{y}_j, \tau'_j)^\dagger$. If all other times but τ_i and τ'_j are the same, there are two cases: if $\tau_i \geq \tau'_j$ we will have to evaluate the contraction

$$\langle \Psi(\mathbf{x}_i, \tau_i) \Psi(\mathbf{y}_j, \tau'_j)^\dagger \rangle;$$

if $\tau_i \leq \tau'_j$ we need to interchange the two operators, which leads to a minus sign hence to

$$-\langle \Psi(\mathbf{y}_j, \tau'_j)^\dagger \Psi(\mathbf{x}_i, \tau_i) \rangle.$$

Both cases can be described by the single formula

$$-G(\mathbf{x}_i, \mathbf{y}_j; \tau_i - \tau'_j).$$

This argument can be extended to all other contractions, justifying the result that

The average value with a non-interacting Hamiltonian of the time-ordered product of Fermi fields is obtained by contracting in all possible ways an annihilation with a creation operator and regarding any contraction as a non-interacting single-particle Green's function. The sign of each product of contractions is $(-1)^n (-1)^L$, where n is the number of annihilation operators, which has to be equal to the number of creation operators, and L is the number of crossings needed to bring each creation operator to the right of the annihilation operator with which it is contracted.

This is the so-called Wick's theorem. For instance

$$\begin{aligned} & -\langle T_\tau \left(\Psi(\mathbf{x}_1, \tau_1) \Psi(\mathbf{x}_2, \tau_2) \Psi(\mathbf{y}_2, \tau'_2)^\dagger \Psi(\mathbf{y}_1, \tau'_1)^\dagger \right) \rangle \\ &= -G^{(0)}(\mathbf{x}_1, \mathbf{y}_1; \tau_1 - \tau'_1) G^{(0)}(\mathbf{x}_2, \mathbf{y}_2; \tau_2 - \tau'_2) + G^{(0)}(\mathbf{x}_1, \mathbf{y}_2; \tau_1 - \tau'_2) G^{(0)}(\mathbf{x}_2, \mathbf{y}_1; \tau_2 - \tau'_1). \end{aligned}$$

In the case of non interacting bosons the Wick's theorem does not hold rigorously. Yet, if we work with a translationally invariant model and if there is no Bose condensation, the Wick's theorem still works, this time without any phase-factor $(-1)^L$, apart from corrections which vanish in the thermodynamic limit.

5.3 Perturbation theory for the single-particle Green's function and Feynmann diagrams

Let us consider the Hamiltonian for free electrons

$$H_0 = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}, \quad (5.23)$$

in the presence of an interaction

$$H_{int} = \frac{1}{2} \sum_{\sigma\sigma'} \int d\mathbf{x} d\mathbf{y} \Psi_\sigma(\mathbf{x})^\dagger \Psi_{\sigma'}(\mathbf{y})^\dagger U(\mathbf{x} - \mathbf{y}) \Psi_{\sigma'}(\mathbf{y}) \Psi_\sigma(\mathbf{x}),$$

which will be our perturbation V . In the S -matrix it appears

$$\begin{aligned} \int d\tau H_{int}(\tau) &= \frac{1}{2} \sum_{\sigma\sigma'} \int d\mathbf{x} d\mathbf{y} \int d\tau \Psi_\sigma(\mathbf{x}, \tau)^\dagger \Psi_{\sigma'}(\mathbf{y}, \tau)^\dagger U(\mathbf{x} - \mathbf{y}) \Psi_{\sigma'}(\mathbf{y}, \tau) \Psi_\sigma(\mathbf{x}, \tau) \\ &= \frac{1}{2} \sum_{\sigma\sigma'} \int d\mathbf{x} d\mathbf{y} \int d\tau d\tau' \Psi_\sigma(\mathbf{x}, \tau)^\dagger \Psi_{\sigma'}(\mathbf{y}, \tau')^\dagger U(\mathbf{x} - \mathbf{y}) \delta(\tau - \tau') \Psi_{\sigma'}(\mathbf{y}, \tau') \Psi_\sigma(\mathbf{x}, \tau) \\ &\equiv \frac{1}{2} \sum_{\sigma\sigma'} \int dx dy \Psi_\sigma(x)^\dagger \Psi_{\sigma'}(y)^\dagger U(x - y) \Psi_{\sigma'}(y) \Psi_\sigma(x), \end{aligned}$$

where we have introduced the multicomponent coordinates $x = (\mathbf{x}, \tau)$, $y = (\mathbf{y}, \tau')$ and by definition

$$U(x - y) = U(\mathbf{x} - \mathbf{y}) \delta(\tau - \tau').$$

Therefore

$$S(\beta) = T_\tau \left[\exp \left(-\frac{1}{2} \sum_{\sigma\sigma'} \int dx_1 dx_2 \Psi_\sigma(x_1)^\dagger \Psi_{\sigma'}(x_2)^\dagger U(x_1 - x_2) \Psi_{\sigma'}(x_2) \Psi_\sigma(x_1) \right) \right].$$

The single-particle Green's function is, as demonstrated previously,

$$G_\sigma(x, y) = -\frac{1}{\langle S(\beta) \rangle} \langle T_\tau (S(\beta) \Psi_\sigma(x) \Psi_\sigma(y)^\dagger) \rangle, \quad (5.24)$$

where the averages are done with the non interacting Hamiltonian. Let us calculate it up to first order in perturbation theory, namely with

$$S(\beta) \simeq S^{(0)}(\beta) + S^{(1)}(\beta) = 1 - \frac{1}{2} \sum_{\sigma\sigma'} \int dx_1 dx_2 \Psi_\sigma(x_1)^\dagger \Psi_{\sigma'}(x_2)^\dagger U(x_1 - x_2) \Psi_{\sigma'}(x_2) \Psi_\sigma(x_1).$$

We need to calculate up to first order the numerator and the denominator of (5.24). About the numerator and using Wick's theorem we find

$$\begin{aligned} -\langle T_\tau (S(\beta) \Psi_\sigma(x) \Psi_\sigma(y)^\dagger) \rangle &= G_\sigma^{(0)}(x, y) \\ &+ \frac{1}{2} \sum_{\alpha\beta} \int dx_1 dx_2 U(x_1 - x_2) \langle T_\tau [\Psi_\sigma(x) \Psi_\sigma(y)^\dagger \Psi_\alpha(x_1)^\dagger \Psi_\beta(x_2)^\dagger \Psi_\beta(x_2) \Psi_\alpha(x_1)] \rangle \\ &= G_\sigma^{(0)}(x, y) \left(1 + \langle S^{(1)}(\beta) \rangle \right) \\ &+ \frac{1}{2} \sum_{\alpha\beta} \int dx_1 dx_2 U(x_1 - x_2) \left[\delta_{\sigma\alpha} G_\sigma^{(0)}(x, x_1) G_\sigma^{(0)}(x_1, y) G_\beta^{(0)}(x_2, x_2) \right. \\ &\quad \left. - \delta_{\sigma\alpha} \delta_{\alpha\beta} G_\sigma^{(0)}(x, x_1) G_\sigma^{(0)}(x_1, x_2) G_\sigma^{(0)}(x_2, y) \right] \end{aligned}$$

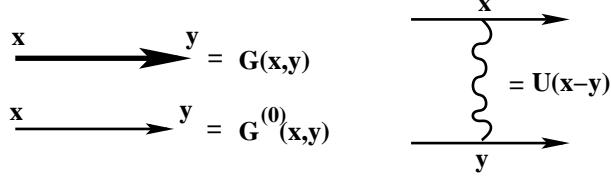


Figure 5.3: Graphical representation of the Green's functions and the interaction.

$$+\frac{1}{2} \sum_{\alpha\beta} \int dx_1 dx_2 U(x_1 - x_2) \left[\delta_{\sigma\beta} G_\sigma^{(0)}(x, x_2) G_\sigma^{(0)}(x_2, y) G_\alpha^{(0)}(x_1, x_1) \right. \\ \left. - \delta_{\sigma\beta} \delta_{\beta\alpha} G_\sigma^{(0)}(x, x_2) G_\sigma^{(0)}(x_2, x_1) G_\beta^{(0)}(x_1, y) \right]$$

The last two integrals are actually equal since we can interchange $x_1 \leftrightarrow x_2$, so that

$$-\langle T_\tau \left(S(\beta) \Psi_\sigma(x) \Psi_\sigma(y)^\dagger \right) \rangle = G_\sigma^{(0)}(x, y) \left(1 + \langle S^{(1)}(\beta) \rangle \right) \\ + \sum_{\alpha\beta} \int dx_1 dx_2 U(x_1 - x_2) \left[\delta_{\sigma\alpha} G_\sigma^{(0)}(x, x_1) G_\sigma^{(0)}(x_1, y) G_\beta^{(0)}(x_2, x_2) \right. \\ \left. - \delta_{\sigma\alpha} \delta_{\alpha\beta} G_\sigma^{(0)}(x, x_1) G_\sigma^{(0)}(x_1, x_2) G_\sigma^{(0)}(x_2, y) \right]$$

The denominator gives simply $1 + \langle S^{(1)}(\beta) \rangle$ so that, up to first order

$$G_\sigma(x, y) = G_\sigma^{(0)}(x, y) + \int dx_1 dx_2 U(x_1 - x_2) \left[G_\sigma^{(0)}(x, x_1) G_\sigma^{(0)}(x_1, y) \sum_\beta G_\beta^{(0)}(x_2, x_2) \right. \\ \left. - G_\sigma^{(0)}(x, x_1) G_\sigma^{(0)}(x_1, x_2) G_\sigma^{(0)}(x_2, y) \right]. \quad (5.25)$$

Let us give a graphical representation of this result. We represent the fully interacting Green's function as a line with an arrow, the non-interacting one as a thin line and the interaction as a wavy line with four legs, see Fig. 5.3. An incoming vertex represent a creation operator, while an outgoing one an annihilation operator. With these notations the Green's function up to first order in the interaction can be represented as in Fig 5.4. The conventions are that any internal coordinate is integrated, the spin is conserved along a Green's function as well as at any interaction-vertex, and a wavy line is the interaction U . There are two first order diagrams. The tadpole one has a plus sign while the other one a minus sign. We notice that both diagrams are fully connected. Actually the disconnected pieces cancel with the denominator $\langle S(\beta) \rangle$. One can go on and calculate the second order corrections to infer the rules for constructing diagrams. Here we just quote the final answer.

The n -th order diagrams for the single particle Green's functions are all fully connected and topologically not equivalent diagrams which can be constructed with n interaction lines and $2n + 1$ non-interacting Green's functions, with external points at x and y . All internal coordinates are integrated. The sign of each diagram is $(-1)^n (-1)^L$, where L is the number of internal loops. Spin is conserved at each vertex, hence each loop implies a spin sum. Finally, if a Green's function is connected by the same interaction line it has to be interpreted as the limit of $\tau \rightarrow 0^-$, since in the interaction creation operators are on the left of the annihilation ones.

One easily realizes that the following rules reproduce the two first order corrections we have just derived.

In Fig. 5.5 we draw all topologically inequivalent diagrams at second order in perturbation theory. Let us follow the above rules to find the expression of the last two, (h) and (i). The former has no loops, hence its sign is simply $(-1)^n = (-1)^2 = 1$. The spin is the same for all lines hence its expression is

$$(h) = \int \prod_{i=1}^4 dx_i U(x_1 - x_3) U(x_2 - x_4) G_\sigma^{(0)}(x, x_1) G_\sigma^{(0)}(x_1, x_2) G_\sigma^{(0)}(x_2, x_3) G_\sigma^{(0)}(x_3, x_4) G_\sigma^{(0)}(x_4, y).$$

Diagram (i) has a loop, hence $(-1)^n (-1)^L = (-1)^2 (-1)^1 = -1$. The internal loop implies a spin summation, hence

$$(i) = - \sum_\beta \int \prod_{i=1}^4 dx_i U(x_1 - x_3) U(x_2 - x_4) G_\sigma^{(0)}(x, x_1) G_\sigma^{(0)}(x_1, x_2) G_\sigma^{(0)}(x_2, y) G_\beta^{(0)}(x_3, x_4) G_\beta^{(0)}(x_4, x_3).$$

5.3.1 Diagram technique in momentum and frequency space

Let us assume that, besides time-translational invariance, the system is also space translational invariant. Therefore let us derive the perturbation expansion of the Fourier transform of the

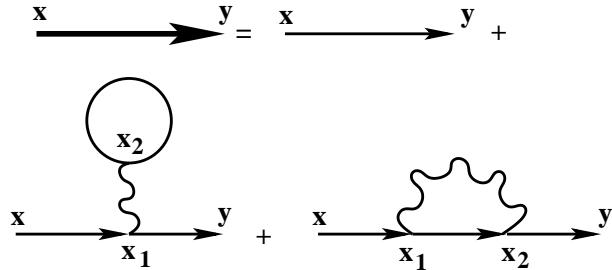


Figure 5.4: Graphical representation of the Green's function up to first order.

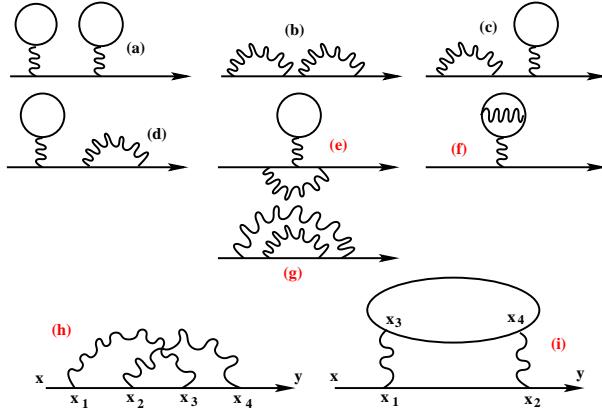


Figure 5.5: Graphical representation of the second order corrections to the Green's function.

Green's function $G_\sigma(\mathbf{p}, i\epsilon_n)$. We further need to introduce the Fourier transform of the interaction line as well as we need to indicate a direction to this line, which is the direction along

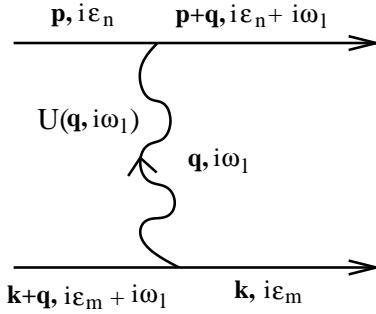


Figure 5.6: Graphical representation of the interaction in Fourier space.

which momentum and frequency flow, see Fig. 5.6. Notice that the frequency carried by the interaction is the difference between two fermionic Matsubara frequencies, hence it is a bosonic one, namely an even multiple of πT . Moreover, since $U(x - y) = U(\mathbf{x} - \mathbf{y}) \delta(\tau - \tau')$, the Fourier transform is $U(\mathbf{q}, i\omega_l) = U(\mathbf{q})$, independent of frequency. Moving to the perturbation expansion, since the spatial and time coordinates of each internal vertex are integrated out, momentum and frequency are conserved at each vertex, namely the sum of the incoming values is equal to that of the outgoing ones. Therefore the rules are:

The n -th order diagrams for the single particle Green's functions with momentum \mathbf{p} and frequency $i\epsilon_n$ are all fully connected and topologically not equivalent diagrams which can be constructed with n interaction lines and $2n+1$ non-interacting Green's functions, with external lines at $(\mathbf{p}, i\epsilon_n)$. At each vertex, the sum of momenta and

that of frequencies of the incoming lines must be equal to the those of outgoing lines. All internal momenta and frequency are summed up, sum over momentum, e.g. \mathbf{k} , being

$$\frac{1}{V} \sum_{\mathbf{k}},$$

and over frequency, e.g. $i\epsilon_m$,

$$T \sum_m.$$

The sign of each diagram is $(-1)^n (-1)^L$, where L is the number of internal loops. Spin is conserved at each vertex, hence each loop implies a spin sum. Finally, if a Green's function is connected by the same interaction line it has to be interpreted as the inverse Fourier transform at $\tau = 0^-$, i.e.

$$T \sum_m G_\sigma(\mathbf{k}, i\epsilon_m) e^{-i\epsilon_m 0^-}.$$

For instance up to first order the diagrams are those in Fig. 5.7 and are explicitly

$$\begin{aligned} G_\sigma(\mathbf{p}, i\epsilon_n) &= G_\sigma^{(0)}(\mathbf{p}, i\epsilon_n) + G_\sigma^{(0)}(\mathbf{p}, i\epsilon_n)^2 U(\mathbf{0}) T \sum_m \frac{1}{V} \sum_{\mathbf{k}} \sum_{\beta} G_\beta^{(0)}(\mathbf{k}, i\epsilon_m) e^{-i\epsilon_m 0^-} \\ &\quad - G_\sigma^{(0)}(\mathbf{p}, i\epsilon_n)^2 T \sum_l \frac{1}{V} \sum_{\mathbf{q}} U(\mathbf{q}) G_\sigma^{(0)}(\mathbf{p} - \mathbf{q}, i\epsilon_n - i\omega_l) e^{-i(\epsilon_n - \omega_l) 0^-}, \end{aligned}$$

where we use the convention that ϵ denote fermionic Matsubara frequencies and ω bosonic ones.

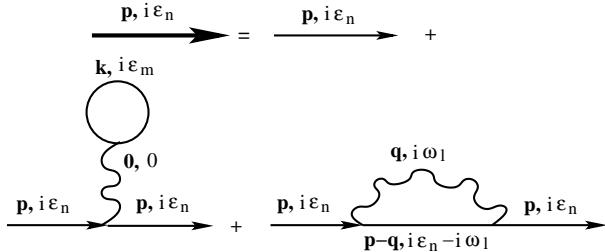


Figure 5.7: Diagrams for the single-particle Green's function up to first order in Fourier space.

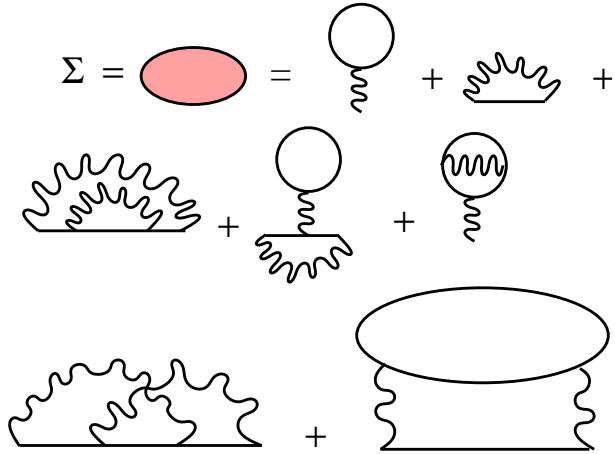


Figure 5.8: Diagrams for the single-particle self-energy up to second order.

5.3.2 The Dyson equation

Among all possible diagrams for the single particle Green's function, we can distinguish two classes. The first includes all diagrams which, by cutting an internal Green's function line, transform in two lower-order diagrams of the same Green's function. These kind of diagrams are called *single-particle reducible*. For instance diagrams (a), (b), (c) and (d) in Fig 5.5 are single-particle reducible. The other class contains all diagrams which are not single-particle reducible, also called *single-particle irreducible*. For instance both first order diagrams as well as the second order ones (e) to (i) are irreducible. Let us for convenience introduce a generalized momentum $p = (\mathbf{p}, i\epsilon_n)$ and let us define as the single-particle self-energy $\Sigma_\sigma(p)$ the sum of all irreducible diagrams without the external legs. For instance, the self-energy diagrams up to second order are drawn in Fig. 5.8, where the self-energy is represented by a rounded box. It

$$\begin{aligned}
 p \rightarrow &= p \rightarrow + p \rightarrow \Sigma(p) p \rightarrow \\
 &+ p \rightarrow \Sigma(p) p \rightarrow \Sigma(p) p \rightarrow + \dots \\
 &= p \rightarrow + p \rightarrow \Sigma(p) p \rightarrow
 \end{aligned}$$

Figure 5.9: Dyson equation for the single-particle Green's function.

is not difficult to realize that, in terms of the self-energy, the perturbation expansion can be

rewritten as in Fig. 5.9, which has the formal solution

$$G_\sigma(\mathbf{p}, i\epsilon_n) = \frac{G_\sigma^{(0)}(\mathbf{p}, i\epsilon_n)}{1 - G_\sigma^{(0)}(\mathbf{p}, i\epsilon_n) \Sigma_\sigma(\mathbf{p}, i\epsilon_n)} = \frac{1}{i\epsilon_n - \epsilon_{\mathbf{p}} - \Sigma(\mathbf{p}, i\epsilon_n)}, \quad (5.26)$$

the last expression being valid for H_0 in Eq. (5.23), which, being spin-independent like the interaction, can not produce two different self-energies for spin-up and down electrons. This is the so-called Dyson equation for the single-particle Green's function. There are therefore two possible ways of doing perturbation theory. The simplest is just to do perturbation theory, say up to order n , directly for the Green's function. The second is to obtain up to order n the self energy and insert its expression in the Dyson equation (5.26). This provides in principle an approximate Green's function which contains all order in perturbation theory, so (5.26) actually represents a way to sum up perturbation theory. This latter is in reality the most physical way to proceed. The reason is that the perturbation is going to change the branch cut singularities of the Green's function, which can be traced easier using (5.26) than directly from the perturbative expansion of G .¹

Physical meaning of the self-energy

The single particle Green's function has a branch cut on the real axis, see (5.14), which implies that the real part is continuous but the imaginary part has a jump. This also means that the real part of the self-energy is continuous but the imaginary part is not, so that we can define

$$\Sigma'(\mathbf{k}, \epsilon) = \mathcal{R}e \Sigma(\mathbf{k}, \epsilon + i\eta) = \mathcal{R}e \Sigma(\mathbf{k}, \epsilon - i\eta),$$

¹A simple way to explain it is the following. Let us take the Green's function for non-interacting fermions

$$G(i\epsilon_n) = \frac{1}{i\epsilon_n - E(V)},$$

where $E(V)$ are the single-particle eigenvalues which depend on some Hamiltonian parameter V , so that

$$E(V=0) = E_0 + \sum_n E_n V^n,$$

and the unperturbed Green's function at $V=0$ is

$$G^{(0)}(i\epsilon_n) = \frac{1}{i\epsilon_n - E_0}.$$

The calculation of the self-energy in perturbation theory gives simply the perturbation expansion of the eigenvalues hence tells us how these eigenvalues changes with V . On the contrary the perturbation expansion of the Green's function

$$G = G^{(0)} + V \left(G^{(0)} \right)^2 E_1 V_1 + V^2 \left(\left(G^{(0)} \right)^2 E_2 + \left(G^{(0)} \right)^3 E_1^2 \right) + \dots,$$

is of difficult interpretation since at each order in perturbation theory all lower order corrections to the eigenvalue intervene.

$$\Sigma''(\mathbf{k}, \epsilon) = \text{Im} \Sigma(\mathbf{k}, \epsilon + i\eta) = -\text{Im} \Sigma(\mathbf{k}, \epsilon - i\eta) \leq 0,$$

where $\eta \rightarrow 0^+$ and the last inequality follows from the fact that the spectral function is positive and given by

$$A(\mathbf{k}, \epsilon) = \frac{1}{\pi} \frac{\eta - \Sigma''(\mathbf{k}, \epsilon)}{(\epsilon - \epsilon_{\mathbf{k}} - \Sigma'(\mathbf{k}, \epsilon))^2 + (\eta - \Sigma''(\mathbf{k}, \epsilon))^2}.$$

For non-interacting electrons $\Sigma = 0$ and the spectral function tends towards a δ -function $\delta(\epsilon - \epsilon_{\mathbf{k}})$ for $\eta \rightarrow 0$. For interacting electrons this δ -function broadens on a width which is controlled by $\Sigma''(\mathbf{k}, \epsilon)$. This broadening reflects the fact that, for instance, a particle, $\epsilon_{\mathbf{k}} > 0$, can decay by the interaction into a particle plus several particle-hole pairs provided that momentum is conserved. The product of this decay will have an energy which is spread around the non-interacting value $\epsilon_{\mathbf{k}}$. Therefore $\Sigma''(\mathbf{k}, \epsilon)$ can be regarded as the decay rate of a particle with momentum \mathbf{k} into an object with the same momentum but energy ϵ . This interpretation can be justified by analyzing the structure of the self-energy diagrams which contribute to the imaginary part. Let us consider for instance the second-order diagram for the self-energy $\Sigma(\mathbf{k}, i\epsilon)$ drawn in Fig. 5.10. Neglecting

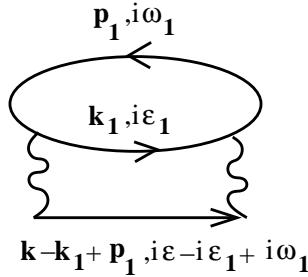


Figure 5.10: Second-order diagram contributing to the imaginary part of the self-energy.

the momentum dependence of the interaction, its expression is

$$\begin{aligned} \delta\Sigma(\mathbf{k}, i\epsilon) = & -2U^2 \frac{1}{V^2} \sum_{\mathbf{k}_0 \mathbf{k}_1 \mathbf{p}_1} T^2 \sum_{\epsilon_1 \omega_1} \delta(\mathbf{k}_0 - \mathbf{k} - \mathbf{p}_1 + \mathbf{k}_1) \\ & \frac{1}{i\epsilon_1 - \epsilon_{\mathbf{k}_1}} \frac{1}{i\omega_1 - \epsilon_{\mathbf{p}_1}} \frac{1}{i\epsilon + i\omega_1 - i\epsilon_1 - \epsilon_{\mathbf{k}_0}}, \end{aligned}$$

where the δ -function imposes the momentum conservation and the factor 2 comes from the loop spin summation. Let us first sum over $i\epsilon_1$, which gives

$$\begin{aligned} T \sum_{\epsilon_1} \frac{1}{i\epsilon_1 - \epsilon_{\mathbf{k}_1}} \frac{1}{i\epsilon + i\omega_1 - i\epsilon_1 - \epsilon_{\mathbf{k}_0}} &= f(\epsilon_{\mathbf{k}_1}) \frac{1}{i\epsilon + i\omega_1 - \epsilon_{\mathbf{k}_1} - \epsilon_{\mathbf{k}_0}} \\ &- f(i\epsilon + i\omega_1 - \epsilon_{\mathbf{k}_0}) \frac{1}{i\epsilon + i\omega_1 - \epsilon_{\mathbf{k}_0} - \epsilon_{\mathbf{k}_1}} \end{aligned}$$

$$= (f(\epsilon_{\mathbf{k}_1}) - f(-\epsilon_{\mathbf{k}_0})) \frac{1}{i\epsilon + i\omega_1 - \epsilon_{\mathbf{k}_0} - \epsilon_{\mathbf{k}_1}},$$

where we used the fact the $i\epsilon + i\omega_1$ is a bosonic frequency. Notice that for $T = 0$ this term is finite only if \mathbf{k}_1 and \mathbf{k}_0 are both particles or holes, namely if $\epsilon_{\mathbf{k}_0}\epsilon_{\mathbf{k}_1} > 0$. Now let us sum over $i\omega_1$,

$$\begin{aligned} T \sum_{\omega_1} \frac{1}{i\omega_1 - \epsilon_{\mathbf{p}_1}} \frac{1}{i\epsilon + i\omega_1 - \epsilon_{\mathbf{k}_0} - \epsilon_{\mathbf{k}_1}} &= f(\epsilon_{\mathbf{p}_1}) \frac{1}{i\epsilon + \epsilon_{\mathbf{p}_1} - \epsilon_{\mathbf{k}_0} - \epsilon_{\mathbf{k}_1}} \\ &\quad + f(\epsilon_{\mathbf{k}_0} + \epsilon_{\mathbf{k}_1} - i\epsilon) \frac{1}{\epsilon_{\mathbf{k}_0} + \epsilon_{\mathbf{k}_1} - i\epsilon - \epsilon_{\mathbf{p}_1}} \\ &= (f(\epsilon_{\mathbf{p}_1}) + b(\epsilon_{\mathbf{k}_0} + \epsilon_{\mathbf{k}_1})) \frac{1}{i\epsilon + \epsilon_{\mathbf{p}_1} - \epsilon_{\mathbf{k}_0} - \epsilon_{\mathbf{k}_1}}. \end{aligned}$$

Here we used the fact that, since $i\epsilon$ is fermionic, then

$$f(\epsilon_{\mathbf{k}_0} + \epsilon_{\mathbf{k}_1} - i\epsilon) = \left(e^{\beta(\epsilon_{\mathbf{k}_0} + \epsilon_{\mathbf{k}_1} - i\epsilon)} + 1 \right) = \left(-e^{\beta(\epsilon_{\mathbf{k}_0} + \epsilon_{\mathbf{k}_1})} + 1 \right) = -b(\epsilon_{\mathbf{k}_0} + \epsilon_{\mathbf{k}_1}).$$

Since at $T = 0$ $b(x) = -\theta(-x)$ and $f(x) = \theta(-x)$, the sum over $i\omega_1$ vanishes if $\epsilon_{\mathbf{p}_1} < 0$ and $\epsilon_{\mathbf{k}_0} + \epsilon_{\mathbf{k}_1} < 0$ or if $\epsilon_{\mathbf{p}_1} > 0$ and $\epsilon_{\mathbf{k}_0} + \epsilon_{\mathbf{k}_1} > 0$. Since $\epsilon_{\mathbf{k}_0}\epsilon_{\mathbf{k}_1} > 0$ for the sum over $i\epsilon_1$ to be finite, the only possibilities are: (1) $\epsilon_{\mathbf{k}_0} > 0$, $\epsilon_{\mathbf{k}_1} > 0$ and $\epsilon_{\mathbf{p}_1} < 0$ or (2) $\epsilon_{\mathbf{k}_0} < 0$, $\epsilon_{\mathbf{k}_1} < 0$ but now $\epsilon_{\mathbf{p}_1} > 0$.

Now we send $i\epsilon \rightarrow \epsilon + i0^+$ with $\epsilon > 0$ and just consider the imaginary part, namely

$$\frac{1}{i\epsilon + \epsilon_{\mathbf{p}_1} - \epsilon_{\mathbf{k}_0} - \epsilon_{\mathbf{k}_1}} \rightarrow \frac{1}{\epsilon + i0^+ + \epsilon_{\mathbf{p}_1} - \epsilon_{\mathbf{k}_0} - \epsilon_{\mathbf{k}_1}} = -i\pi\delta(\epsilon + \epsilon_{\mathbf{p}_1} - \epsilon_{\mathbf{k}_0} - \epsilon_{\mathbf{k}_1}).$$

The δ -function implies that

$$\epsilon_{\mathbf{k}_0} + \epsilon_{\mathbf{k}_1} - \epsilon_{\mathbf{p}_1} = \epsilon > 0,$$

which is only compatible with the above possibility (1), i.e. $\epsilon_{\mathbf{k}_0} > 0$, $\epsilon_{\mathbf{k}_1} > 0$ and $\epsilon_{\mathbf{p}_1} < 0$, thus leading to

$$\mathcal{I}m \delta\Sigma(\mathbf{k}, \epsilon + i0^+) = -2\pi iU^2 \frac{1}{V^2} \sum_{\mathbf{k}_0 \mathbf{k}_1 \mathbf{p}_1} \delta(\mathbf{k}_0 - \mathbf{k} - \mathbf{p}_1 + \mathbf{k}_1) \delta(\epsilon + \epsilon_{\mathbf{p}_1} - \epsilon_{\mathbf{k}_0} - \epsilon_{\mathbf{k}_1}) f(-\epsilon_{\mathbf{k}_1}) f(-\epsilon_{\mathbf{k}_0}) f(\epsilon_{\mathbf{p}_1}).$$

This expression coincides with the Fermi golden rule for the probability of a particle at momentum \mathbf{k} to decay into two particles and one hole with the same total momentum but energy ϵ .

More generally, the diagrams which contribute to the imaginary part of the self-energy can be represented as in Fig. 5.11, where a particle with momentum \mathbf{k} and frequency $i\epsilon$ decays by

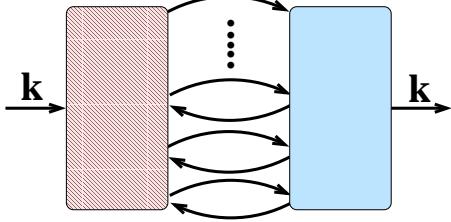


Figure 5.11: Graphical representation of a self-energy diagram which contribute to the imaginary part.

a matrix element drawn as a box into a particle plus a certain number, say $m \geq 1$, of particle-hole pairs,² which recombine through the other box into the original particle. Let us neglect for simplicity the momentum and frequency dependence of the boxes, and define as $\mathbf{k}_i(\epsilon_i)$ and $\mathbf{p}_i(\omega_i)$, $i = 1, m$, the momenta(frequencies) of the particles and holes, respectively, of the m particle-hole pairs, and as $\mathbf{k}_0(\epsilon_0)$ that of the additional particle. By momentum and frequency conservation

$$\mathbf{k}_0 + \sum_i \mathbf{k}_i - \mathbf{p}_i = \mathbf{k}, \quad \epsilon_0 + \sum_i \epsilon_i - \omega_i = \epsilon_n.$$

As before, if we sum over all the $2m$ independent internal frequencies and finally send $i\epsilon \rightarrow \epsilon + i0^+$, with $\epsilon > 0$, we end up with expression for the imaginary part proportional to

$$\sum_{\mathbf{k}_0} \sum_{\mathbf{k}_i \mathbf{p}_i} \delta\left(\epsilon - \sum_j (\epsilon_{\mathbf{k}_j} - \epsilon_{\mathbf{p}_j}) - \epsilon_{\mathbf{k}_0}\right) \delta\left(\mathbf{k}_0 + \sum_j (\mathbf{k}_j - \mathbf{p}_j) - \mathbf{k}\right) f(-\epsilon_{\mathbf{k}_0}) \prod_{j=1}^m f(-\epsilon_{\mathbf{k}_j}) f(\epsilon_{\mathbf{p}_j}).$$

Since $\epsilon_{\mathbf{k}_i} \geq 0$ and $\epsilon_{\mathbf{p}_i} \leq 0$, the energy conservation implies that, for small ϵ , all particles and holes should lie very close to the Fermi surface, on a strip of width at most $\delta k = \epsilon/v_F$, where v_F is the Fermi velocity. Therefore the phase space available for the decay process grows at most like ϵ^{2m} , since there are only $2m$ free summations over momentum, \mathbf{k}_0 being fixed by momentum conservation.

The final conclusion is therefore that, within perturbation theory,

$$\lim_{\epsilon \rightarrow 0} \Sigma''(\mathbf{k}, \epsilon) = \lim_{\epsilon \rightarrow 0} \text{Im} \Sigma(\mathbf{k}, \epsilon + i\eta) = 0, \quad (5.27)$$

²Two lines which propagate in opposite directions correspond to two Green's functions one at positive time and the other at negative time. Positive time means that first we create an electron and later we annihilate it, which denote a so-called particle excitation. On the contrary, negative time means that first we annihilate an electron and later we create it back, so-called hole excitation.

5.4 Other kinds of perturbations

So far we have just constructed and analysed the perturbation expansion in terms of the electron-electron interaction. Let us consider now what changes for different types of perturbations. In particular we will just briefly mention two perturbations: a scalar potential and the coupling to bosonic modes.

5.4.1 Scalar potential

Let us suppose to have non-interacting electrons identified by a quantum label a , with non-interacting Green's functions

$$G_{ab}^{(0)}(\mathbf{x}, \mathbf{y}; \tau) = \delta_{ab} G_a^{(0)}(\mathbf{x}, \mathbf{y}; \tau),$$

in the presence of the scalar potential

$$V = \sum_{ab} \int d\mathbf{x} \Psi_a(\mathbf{x}) V(\mathbf{x})_{ab} \Psi_b(\mathbf{x}). \quad (5.28)$$

The S -matrix is now

$$\begin{aligned} S(\beta) &= T_\tau \left(\exp \left(- \sum_{ab} \int_0^\beta d\tau \int d\mathbf{x} \Psi_a(\mathbf{x}, \tau) V(\mathbf{x})_{ab} \Psi_b(\mathbf{x}, \tau) \right) \right) \\ &\equiv T_\tau \left(\exp \left(- \sum_{ab} \int dx \Psi_a(x) V(x)_{ab} \Psi_b(x) \right) \right), \end{aligned}$$

where, as before, we have introduced the four-dimensional coordinate $x = (\mathbf{x}, \tau)$. Upon expanding $S(\beta)$ up to first order and keeping only connected diagrams, one can readily obtain the Green's function expansion

$$\begin{aligned} G_{ab}(x, y) &= \delta_{ab} G_a^{(0)}(x, y) + \sum_{cd} \int dz V(z)_{cd} \langle T_\tau \left(\Psi_a(x) \Psi_b(y)^\dagger \Psi_c(z)^\dagger \Psi_d(z) \right) \rangle_{conn} \\ &= \delta_{ab} G_a^{(0)}(x, y) + \int dz V(z)_{ab} G_a^{(0)}(x, z) G_b^{(0)}(z, y). \end{aligned} \quad (5.29)$$

If we represent graphically the perturbation as in Fig. 5.12(a), then the Green's function (5.29) up to first order can be drawn as the first two diagrams in the right hand side of Fig. 5.12(b). Higher order terms can be simply obtained by inserting other potential lines, as the second order term in Fig. 5.12(b). All diagrams have a positive sign. The Dyson equation can be easily read out:

$$G_{ab}(x, y) = \delta_{ab} G_a^{(0)}(x, y) + \sum_c \int dz V(z)_{ac} G_a^{(0)}(x, z) G_{cb}(z, y), \quad (5.30)$$

and is drawn in Fig. 5.12(b).

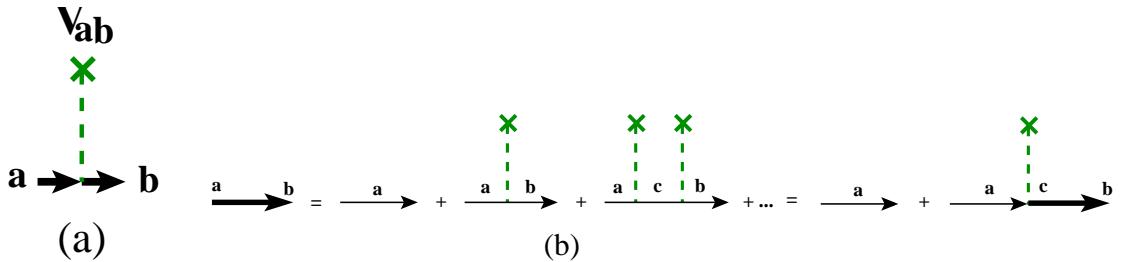


Figure 5.12: (a) Graphical representation of the scalar potential perturbation. (b) Perturbation expansion of the Green's function and Dyson equation.

5.4.2 Coupling to bosonic modes

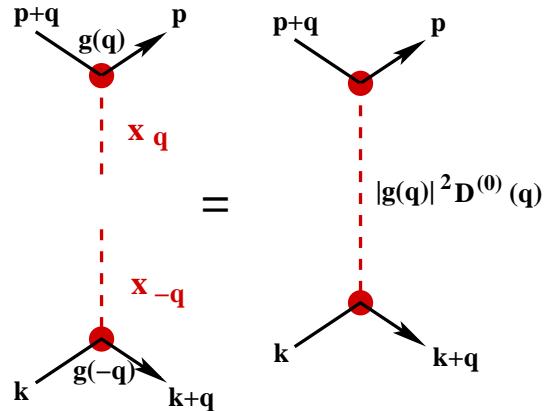


Figure 5.13: On the left: electron-phonon vertices at \mathbf{q} and $-\mathbf{q}$. The external dotted vertex line represents phonon coordinates. On the right: the effective electron-electron interaction after contracting phonons.

Let us imagine now that our system of electrons is coupled to phonons described by the free Hamiltonian

$$H_{phon} = \sum_{\mathbf{q}} \omega_{\mathbf{q}} a_{\mathbf{q}}^\dagger a_{\mathbf{q}}.$$

The coupling term is assumed to be

$$V = \sum_{\mathbf{q}} g(\mathbf{q}) x_{\mathbf{q}} \rho(-\mathbf{q}), \quad (5.31)$$

where $g(\mathbf{q})^* = g(-\mathbf{q})$ is the coupling constant, the phonon coordinate is

$$x_{\mathbf{q}} = \sqrt{\frac{1}{2}} (a_{\mathbf{q}} + a_{-\mathbf{q}}^\dagger),$$

and

$$\rho(\mathbf{q}) = \sum_{\sigma} \sum_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}+\mathbf{q}\sigma},$$

is the density operator. This perturbation is actually more general and describes any kind of electron-boson coupling.

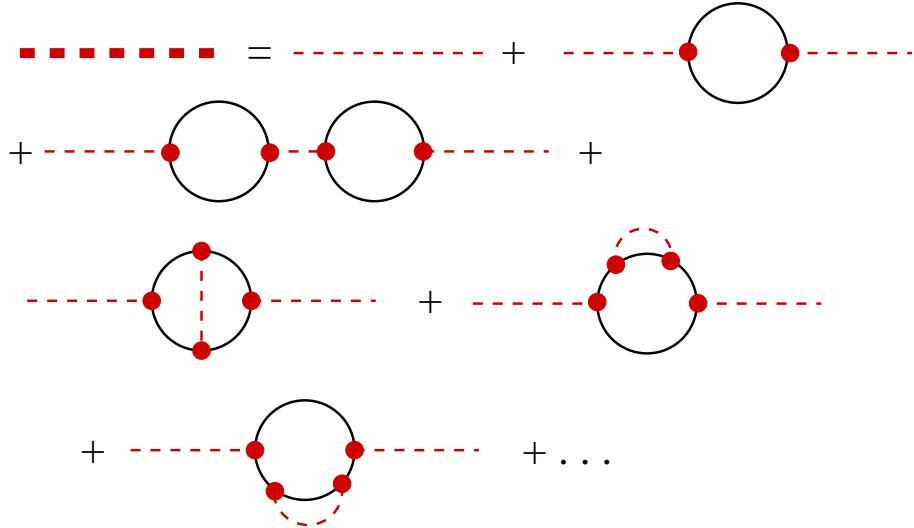


Figure 5.14: First orders in the diagrammatic perturbation expansion of $D(q)$. The exact $D(q)$ is represented by a bold dashed line, while $D^{(0)}(q)$ by a thinner dashed line. The solid lines are electron Green's functions.

We can perform perturbation theory in (5.31) using the Wick theorem both for the electrons and for the bosons. The latter amounts to contract an $x_{\mathbf{q}}$ with $x_{-\mathbf{q}}$ which leads to the free propagator $D^{(0)}(\mathbf{q}, i\omega_n)$ of Eq. (5.19). Therefore, if we represent the electron-phonon coupling as in Fig. 5.13, in which a dotted vertex line represents the phonon-coordinate, by contracting two vertices one recovers an effective electron-electron interaction, see also Fig. 5.13, which is mediated by the phonons and given by

$$|g(\mathbf{q})|^2 D^{(0)}(\mathbf{q}, i\omega_l) = -|g(\mathbf{q})|^2 \frac{\omega_{\mathbf{q}}}{\omega_l^2 + \omega_{\mathbf{q}}^2}. \quad (5.32)$$

This effective interaction is retarded, namely depends on the frequency, and attractive. More specifically, if we move on the real axis, then

$$|g(\mathbf{q})|^2 D^{(0)}(\mathbf{q}, i\omega_l \rightarrow \omega) \rightarrow -|g(\mathbf{q})|^2 \frac{\omega_{\mathbf{q}}}{\omega_{\mathbf{q}}^2 - \omega^2},$$

which is attractive if $|\omega| < \omega_q$ and repulsive otherwise. The rules for constructing diagrams are therefore the same as for the electron-electron interaction, with the additional complication that interaction is frequency dependent.

However, in this particular case one may also investigate the effects of the electron-phonon coupling to the phonon Green's function $D(\mathbf{q}, i\omega_l)$. The perturbation expansion is shown up to second order in Fig. 5.14. Two kinds of diagrams can be identified. The first class includes diagrams which can be divided into two diagrams of the same expansion by cutting non-interacting $D^{(0)}(q)$ -line, like the first second order diagram shown in Fig. 5.14. These diagrams are reducible. The other class includes all other diagrams which are irreducible. If we define a self-energy $|g(\mathbf{q})|^2 \Pi(\mathbf{q}, i\omega_n)$ through these irreducible diagrams, shown up to second order in Fig. 5.15, we can easily derive the Dyson equation, also shown in the same figure, whose solution is

$$D(\mathbf{q}, i\omega_n) = \frac{D^{(0)}(\mathbf{q}, i\omega_n)}{1 - |g(\mathbf{q})|^2 D^{(0)}(\mathbf{q}, i\omega_n) \Pi(\mathbf{q}, i\omega_n)}. \quad (5.33)$$

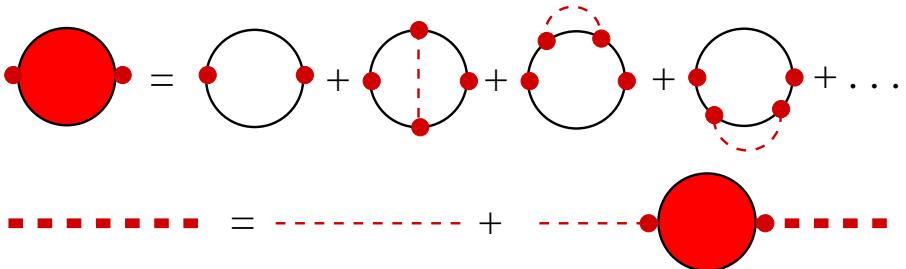


Figure 5.15: Upper panel: Phonon self-energy, represented by a filled circle, up to second order. Lower panel: Dyson equation for $D(q)$.

5.5 Two-particle Green's functions and correlation functions

Let us consider back the Hamiltonian of interacting electrons, which we assumed to be

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \frac{1}{2V} \sum_{\mathbf{k}\mathbf{p}\mathbf{q}} \sum_{\alpha\beta} U(\mathbf{q}) c_{\mathbf{p}\alpha}^\dagger c_{\mathbf{k}+\mathbf{q}\beta}^\dagger c_{\mathbf{k}\beta} c_{\mathbf{p}+\mathbf{q}\alpha}. \quad (5.34)$$

The Heisenberg imaginary time evolution of an annihilation operator is

$$\begin{aligned} -\frac{\partial c_{\mathbf{k}\sigma}(\tau)}{\partial \tau} &= [c_{\mathbf{k}\sigma}(\tau), H(\tau)] = \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}(\tau) \\ &\quad + \frac{1}{V} \sum_{\mathbf{p}\mathbf{q}\alpha} U(\mathbf{q}) c_{\mathbf{p}+\mathbf{q}\alpha}^\dagger(\tau) c_{\mathbf{p}\alpha}(\tau) c_{\mathbf{k}+\mathbf{q}\sigma}(\tau). \end{aligned}$$

Therefore the Green's function satisfies the equation of motion

$$\begin{aligned} -\frac{\partial}{\partial \tau} G_\sigma(\mathbf{k}, \tau) &= -\frac{\partial}{\partial \tau} \left[-\langle T_\tau \left(c_{\mathbf{k}\sigma}(\tau) c_{\mathbf{k}\sigma}^\dagger \right) \rangle \right] \\ &= -\frac{\partial}{\partial \tau} \left[-\theta(\tau) \langle c_{\mathbf{k}\sigma}(\tau) c_{\mathbf{k}\sigma}^\dagger \rangle + \theta(-\tau) \langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}(\tau) \rangle \right] \\ &= \delta(\tau) - \langle T_\tau \left(\frac{\partial c_{\mathbf{k}\sigma}(\tau)}{\partial \tau} c_{\mathbf{k}\sigma}^\dagger \right) \rangle \\ &= \delta(\tau) + \epsilon_{\mathbf{k}} G_\sigma(\mathbf{k}, \tau) - \frac{1}{V} \sum_{\mathbf{p}\mathbf{q}\alpha} U(\mathbf{q}) \langle T_\tau \left(c_{\mathbf{p}+\mathbf{q}\alpha}^\dagger(\tau) c_{\mathbf{p}\alpha}(\tau) c_{\mathbf{k}+\mathbf{q}\sigma}(\tau) c_{\mathbf{k}\sigma}^\dagger \right) \rangle. \end{aligned}$$

This equation can be written as

$$\left(-\frac{\partial}{\partial \tau'} - \epsilon_{\mathbf{k}} \right) G_\sigma(\mathbf{k}, \tau') = \delta(\tau') - \frac{1}{V} \sum_{\mathbf{p}\mathbf{q}\alpha} U(\mathbf{q}) \langle T_\tau \left(c_{\mathbf{p}+\mathbf{q}\alpha}^\dagger(\tau') c_{\mathbf{p}\alpha}(\tau') c_{\mathbf{k}+\mathbf{q}\sigma}(\tau') c_{\mathbf{k}\sigma}^\dagger \right) \rangle. \quad (5.35)$$

The non-interacting Green's function satisfies on the contrary

$$\left(-\frac{\partial}{\partial \tau'} - \epsilon_{\mathbf{k}} \right) G_\sigma^{(0)}(\mathbf{k}, \tau') = \delta(\tau').$$

If we multiply both sides of Eq. (5.35) by $G_\sigma^{(0)}(\mathbf{k}, \tau - \tau')$ and integrate over τ' , we obtain

$$\begin{aligned} &\int d\tau' G_\sigma^{(0)}(\mathbf{k}, \tau - \tau') \left(-\frac{\partial}{\partial \tau'} - \epsilon_{\mathbf{k}} \right) G_\sigma(\mathbf{k}, \tau') = G_\sigma^{(0)}(\mathbf{k}, \tau) \\ &- \frac{1}{V} \sum_{\mathbf{p}\mathbf{q}\alpha} U(\mathbf{q}) \int d\tau' G_\sigma^{(0)}(\mathbf{k}, \tau - \tau') \langle T_\tau \left(c_{\mathbf{p}+\mathbf{q}\alpha}^\dagger(\tau') c_{\mathbf{p}\alpha}(\tau') c_{\mathbf{k}+\mathbf{q}\sigma}(\tau') c_{\mathbf{k}\sigma}^\dagger \right) \rangle, \end{aligned}$$

and upon integrating by part the left hand side, one obtains

$$G_\sigma(\mathbf{k}, \tau) = G_\sigma^{(0)}(\mathbf{k}, \tau) - \frac{1}{V} \sum_{\mathbf{pq}\alpha} U(\mathbf{q}) \int d\tau' G_\sigma^{(0)}(\mathbf{k}, \tau - \tau') \langle T_\tau \left(c_{\mathbf{p}+\mathbf{q}\alpha}^\dagger(\tau') c_{\mathbf{p}\alpha}(\tau') c_{\mathbf{k}+\mathbf{q}\sigma}(\tau') c_{\mathbf{k}\sigma}^\dagger(\tau') \right) \rangle. \quad (5.36)$$

Therefore the single-particle Green's function can be expressed in terms of a two-particle Green's function. Namely, let us define the two-particle Green's function

$$K_{\sigma_1\sigma_2;\sigma_3\sigma_4}(\mathbf{p}_1\tau_1, \mathbf{p}_2\tau_2; \mathbf{p}_3\tau_3, \mathbf{p}_4\tau_4) = -\langle T_\tau \left(c_{\mathbf{p}_1\sigma_1}(\tau_1) c_{\mathbf{p}_2\sigma_2}(\tau_2) c_{\mathbf{p}_3\sigma_3}^\dagger(\tau_3) c_{\mathbf{p}_4\sigma_4}^\dagger(\tau_4) \right) \rangle, \quad (5.37)$$

where, by momentum conservation,

$$\mathbf{p}_1 + \mathbf{p}_2 = \mathbf{p}_3 + \mathbf{p}_4,$$

in terms of which

$$G_\sigma(\mathbf{k}, \tau) = G_\sigma^{(0)}(\mathbf{k}, \tau) - \frac{1}{V} \sum_{\mathbf{pq}\alpha} U(\mathbf{q}) \int d\tau G_\sigma^{(0)}(\mathbf{k}, \tau - \tau') K_{\sigma\alpha;\alpha\sigma}(\mathbf{k} + \mathbf{q}\tau', \mathbf{p}\tau'; \mathbf{p} + \mathbf{q}\tau', \mathbf{k}0). \quad (5.38)$$

5.5.1 Diagrammatic representation of the two-particle Green's function

Let us write formally

$$\begin{aligned} K_{\sigma_1\sigma_2;\sigma_3\sigma_4}(\mathbf{p}_1\tau_1, \mathbf{p}_2\tau_2; \mathbf{p}_3\tau_3, \mathbf{p}_4\tau_4) &= -\delta_{\sigma_1\sigma_4} \delta_{\sigma_2\sigma_3} \delta_{\mathbf{p}_1\mathbf{p}_4} \delta_{\mathbf{p}_2\mathbf{p}_3} G_{\sigma_1}(\mathbf{p}_1, \tau_1 - \tau_4) G_{\sigma_2}(\mathbf{p}_2, \tau_2 - \tau_3) \\ &\quad + \delta_{\sigma_1\sigma_3} \delta_{\sigma_2\sigma_4} \delta_{\mathbf{p}_1\mathbf{p}_3} \delta_{\mathbf{p}_2\mathbf{p}_4} G_{\sigma_1}(\mathbf{p}_1, \tau_1 - \tau_3) G_{\sigma_2}(\mathbf{p}_2, \tau_2 - \tau_4) \\ &\quad + \int \prod_{i=1}^4 d\tau'_i G_{\sigma_1}(\mathbf{p}_1, \tau_1 - \tau'_1) G_{\sigma_2}(\mathbf{p}_1, \tau_2 - \tau'_2) G_{\sigma_3}(\mathbf{p}_3, \tau'_3 - \tau_3) G_{\sigma_4}(\mathbf{p}_4, \tau'_4 - \tau_4) \\ &\quad \Gamma_{\sigma_1\sigma_2;\sigma_3\sigma_4}(\mathbf{p}_1\tau'_1, \mathbf{p}_2\tau'_2; \mathbf{p}_3\tau'_3, \mathbf{p}_4\tau'_4), \end{aligned} \quad (5.39)$$

which is represented graphically to Fig. 5.16. We notice that, in the absence of interaction, only the first two terms survive with the Green's functions being the non-interacting ones. If we start doing perturbation theory, which has the same rules as before, we will (1) dress the non-interacting Green's functions, which explains the first two terms; (2) couple them by interaction lines, which justify the last contribution and provides the definition of the interaction vertex Γ , which in lowest order perturbation theory is shown in Fig. 5.17.

In conclusion the equation (5.38) of the single particle Green's function in terms of the two-particle one can be expressed as function of the single particle Green's function itself and the interaction vertex as shown in Fig. 5.18. Notice that the interaction vertex acts as the bare interaction, so it carries a (-1) sign. Since there is a loop in the third diagram of Fig. 5.18, the overall sign is plus. This result also provides an expression for the single-particle self-energy, as shown in Fig. 5.19.

$$\mathbf{K}(1,2;3,4) = - \begin{array}{c} 1 \longrightarrow 4 \\ 2 \longrightarrow 3 \end{array} + \begin{array}{c} 1 \longrightarrow 4 \\ 2 \longrightarrow 3 \end{array}$$

$$+ \begin{array}{c} 1 \longrightarrow 4 \\ 2 \longrightarrow 3 \end{array} \quad \Gamma(1,2;3,4)$$

Figure 5.16: Graphical representation of the two-particle Green's function.

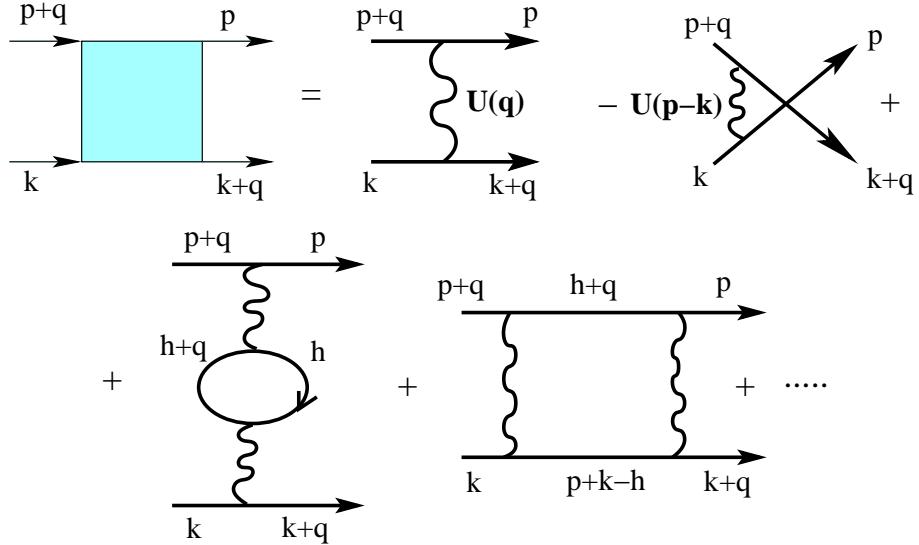


Figure 5.17: Lowest order expansion of the interaction vertex. p , k , $p + q$ and $k + q$ label both momenta and frequencies.

5.5.2 Correlation functions

We already showed that the average value of the imaginary-time ordered product of two bosonic-like operators can provide, after analytic continuation on the real axis, the linear response functions. Let us then consider two single-particle density operators:

$$A(\mathbf{q}) = \sum_{\mathbf{k}\alpha\beta} \lambda_{\mathbf{k},\mathbf{k}+\mathbf{q};\alpha\beta}^A c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}+\mathbf{q}\beta}, \quad B(\mathbf{q}) = \sum_{\mathbf{k}\alpha\beta} \lambda_{\mathbf{k},\mathbf{k}+\mathbf{q};\alpha\beta}^B c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}+\mathbf{q}\beta}.$$

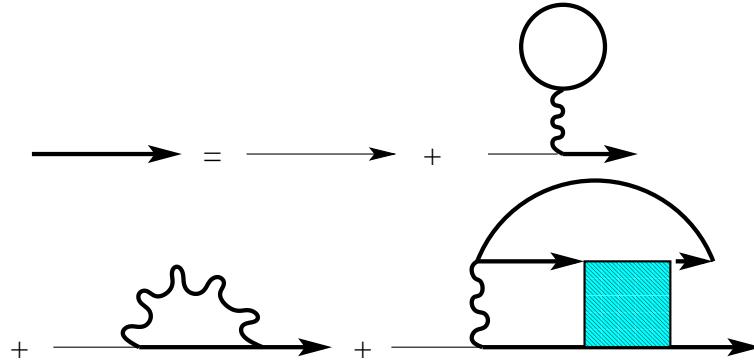


Figure 5.18: Dyson equation in terms of the interaction vertex Γ .

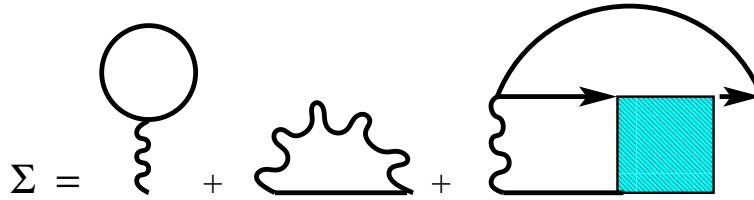


Figure 5.19: Single-particle self-energy in terms of the interaction vertex Γ .

Their Green's function, usually called correlation function, is (we use the notation $G_{AB} = \chi_{AB}$ since we know that the two coincide on the frequency real axis):³

$$\begin{aligned}
\chi_{AB}(\mathbf{q}, \tau) &= -\frac{1}{V} \langle T_\tau (A(\mathbf{q}, \tau) B(-\mathbf{q})) \rangle = -\frac{1}{V} \sum_{\mathbf{k} \alpha \beta} \sum_{\mathbf{p} \gamma \delta} \lambda_{\mathbf{k}, \mathbf{k} + \mathbf{q}; \alpha \beta}^A \lambda_{\mathbf{p} + \mathbf{q}, \mathbf{p}; \gamma \delta}^B \\
&\quad \langle T_\tau (c_{\mathbf{k}\alpha}^\dagger(\tau) c_{\mathbf{k} + \mathbf{q}\beta}(\tau) c_{\mathbf{p} + \mathbf{q}\gamma}^\dagger c_{\mathbf{p}\delta}) \rangle \\
&= \frac{1}{V} \sum_{\mathbf{k} \alpha \beta} \sum_{\mathbf{p} \gamma \delta} \lambda_{\mathbf{k}, \mathbf{k} + \mathbf{q}; \alpha \beta}^A \lambda_{\mathbf{p} + \mathbf{q}, \mathbf{p}; \gamma \delta}^B K_{\beta \delta; \gamma \alpha}(\mathbf{k} + \mathbf{q} \tau, \mathbf{p} 0; \mathbf{p} + \mathbf{q} 0, \mathbf{k} \tau) \\
&= -\frac{1}{V} \left(\sum_{\mathbf{k} \alpha} \lambda_{\mathbf{k}, \mathbf{k}; \alpha \alpha}^A G_\alpha(\mathbf{k}, 0^-) \right) \left(\sum_{\mathbf{p} \gamma} \lambda_{\mathbf{p} + \mathbf{q}; \gamma \gamma}^B G_\gamma(\mathbf{p}, 0^-) \right) \\
&\quad + \frac{1}{V} \sum_{\mathbf{k} \alpha \gamma} \lambda_{\mathbf{k}, \mathbf{k} + \mathbf{q}; \alpha \gamma}^A \lambda_{\mathbf{k} + \mathbf{q}, \mathbf{k}; \gamma \alpha}^B G_\alpha(\mathbf{k} + \mathbf{q}, \tau) G_\gamma(\mathbf{k}, -\tau)
\end{aligned}$$

³In the equation the Green's functions at equal times have to be interpreted as the limit of $\tau \rightarrow 0^-$, since in the definition of A and B creation operators are on the left of the annihilation ones.

$$\begin{aligned}
& + \frac{1}{V} \sum_{\mathbf{k} \alpha \gamma} \lambda_{\mathbf{k}, \mathbf{k}+\mathbf{q}; \alpha \gamma}^A \lambda_{\mathbf{k}+\mathbf{q}, \mathbf{k}; \gamma \alpha}^B \int \prod_{i=1}^4 d\tau_i G_\beta(\mathbf{k} + \mathbf{q}, \tau - \tau_1) G_\delta(\mathbf{p}, 0 - \tau_2) \\
& \quad G_\gamma(\mathbf{p} + \mathbf{q}, \tau_3 - 0) G_\alpha(\mathbf{k}, \tau_4 - \tau) \Gamma_{\beta \delta; \gamma \alpha}(\mathbf{k} + \mathbf{q}, \tau - \tau_1, \mathbf{p} - \tau_2; \mathbf{p} + \mathbf{q}, \tau_3, \mathbf{k}, \tau_4 - \tau) \\
= & - \frac{1}{V} \langle A(\mathbf{q}) \rangle \langle B(-\mathbf{q}) \rangle \\
& + \frac{1}{V} \sum_{\mathbf{k} \alpha \gamma} \lambda_{\mathbf{k}, \mathbf{k}+\mathbf{q}; \alpha \gamma}^A \lambda_{\mathbf{k}+\mathbf{q}, \mathbf{k}; \gamma \alpha}^B G_\alpha(\mathbf{k} + \mathbf{q}, \tau) G_\gamma(\mathbf{k}, -\tau) \\
& + \frac{1}{V} \sum_{\mathbf{k} \alpha \gamma} \lambda_{\mathbf{k}, \mathbf{k}+\mathbf{q}; \alpha \gamma}^A \lambda_{\mathbf{k}+\mathbf{q}, \mathbf{k}; \gamma \alpha}^B \int \prod_{i=1}^4 d\tau_i G_\beta(\mathbf{k} + \mathbf{q}, \tau - \tau_1) G_\delta(\mathbf{p}, 0 - \tau_2) \\
& \quad G_\gamma(\mathbf{p} + \mathbf{q}, \tau_3 - 0) G_\alpha(\mathbf{k}, \tau_4 - \tau) \Gamma_{\beta \delta; \gamma \alpha}(\mathbf{k} + \mathbf{q}, \tau - \tau_1, \mathbf{p} - \tau_2; \mathbf{p} + \mathbf{q}, \tau_3, \mathbf{k}, \tau_4 - \tau).
\end{aligned}$$

The disconnected term $\langle A(\mathbf{q}) \rangle \langle B(-\mathbf{q}) \rangle$ vanishes for $\mathbf{q} \neq \mathbf{0}$. In general it can be moved on the left hand side, in which case the correlation function is the average of the time-ordered product minus the product of the averages. With this definition, the correlation function has the graphical representation shown in Fig. 5.20. In the figure, the triangular vertices represent

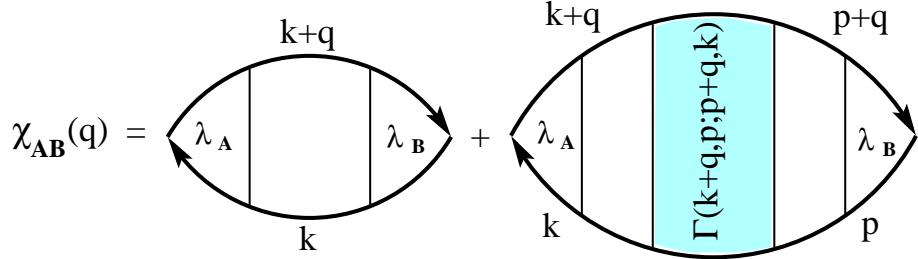


Figure 5.20: Graphical representation of the correlation function $\chi_{AB}(q)$, where q includes both momentum \mathbf{q} and a bosonic frequency $i\omega_l$.

the matrix elements $\lambda_{\mathbf{k}, \mathbf{k}+\mathbf{q}; \alpha \gamma}^{A(B)}$ and the loops imply as usual summation over the spin-indices. Perturbation theory has the same rules as before with the only exception that the loop phase-factor is now $(-1)^{L-1}$ due to the minus sign in the definition of χ . If we Fourier transform also in imaginary time, the correlation function

$$\chi_{AB}(\mathbf{q}, i\omega_l),$$

depends on the transferred momentum, \mathbf{q} , and frequency, $i\omega_l$. Since the operators are bosonic-like, $i\omega_l$ is a bosonic Matsubara frequency. By time-translation invariance, the frequency is conserved at any vertex, as usual, and the interaction vertex becomes consequently

$$\Gamma_{\beta \delta; \gamma \alpha}(\mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l, \mathbf{p}, i\epsilon_m; \mathbf{p} + \mathbf{q}, i\epsilon_m + i\omega_l, \mathbf{k}, i\epsilon_n), \quad (5.40)$$

as shown in Fig. 5.21.

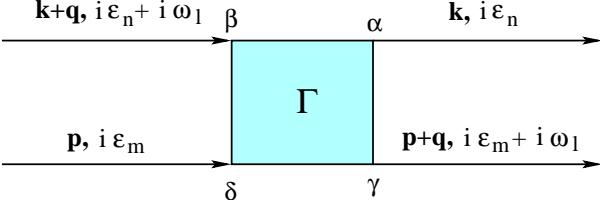


Figure 5.21: Graphical representation of the interaction vertex of Eq. (5.40).

Non-interacting values

In the absence of interaction only the first term in Fig. 5.20 survives with the Green's function lines being the non-interacting ones. Since there is a loop, according to what we said before, the sign is $(-1)^{L-1} = (-1)^{1-1} = 1$ hence

$$\begin{aligned}\chi_{AB}^{(0)}(\mathbf{q}, i\omega_l) &= \frac{1}{V} \sum_{\mathbf{k}} T \sum_n \sum_{\alpha\gamma} \lambda_{\mathbf{k}, \mathbf{k}+\mathbf{q}; \alpha\gamma}^A \lambda_{\mathbf{k}+\mathbf{q}, \mathbf{k}; \gamma\alpha}^B G_{\alpha}^{(0)}(\mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l) G_{\gamma}^{(0)}(\mathbf{k}, i\epsilon_n) \\ &= \frac{1}{V} \sum_{\mathbf{k}} T \sum_n \sum_{\alpha\gamma} \lambda_{\mathbf{k}, \mathbf{k}+\mathbf{q}; \alpha\gamma}^A \lambda_{\mathbf{k}+\mathbf{q}, \mathbf{k}; \gamma\alpha}^B \frac{1}{i\epsilon_n + i\omega_l - \epsilon_{\mathbf{k}+\mathbf{q}}} \frac{1}{i\epsilon_n - \epsilon_{\mathbf{k}}}.\end{aligned}\quad (5.41)$$

By means of Eq. (5.8) we can easily perform the sum over frequencies in Eq. (5.41), which gives

$$\begin{aligned}T \sum_n \frac{1}{i\epsilon_n + i\omega_l - \epsilon_{\mathbf{k}+\mathbf{q}}} \frac{1}{i\epsilon_n - \epsilon_{\mathbf{k}}} &= f(\epsilon_{\mathbf{k}+\mathbf{q}} - i\omega_l) \frac{1}{\epsilon_{\mathbf{k}+\mathbf{q}} - i\omega_l - \epsilon_{\mathbf{k}}} + f(\epsilon_{\mathbf{k}}) \frac{1}{i\omega_l - \epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}}} \\ &= \frac{f(\epsilon_{\mathbf{k}}) - f(\epsilon_{\mathbf{k}+\mathbf{q}})}{i\omega_l - \epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}}},\end{aligned}$$

where we used the fact that, if $i\omega_l$ is bosonic, then $f(\epsilon \pm i\omega_l) = f(\epsilon)$. The final result is therefore

$$\chi_{AB}^{(0)}(\mathbf{q}, i\omega_l) = \frac{1}{V} \sum_{\mathbf{k}} \sum_{\alpha\gamma} \lambda_{\mathbf{k}, \mathbf{k}+\mathbf{q}; \alpha\gamma}^A \lambda_{\mathbf{k}+\mathbf{q}, \mathbf{k}; \gamma\alpha}^B \frac{f(\epsilon_{\mathbf{k}}) - f(\epsilon_{\mathbf{k}+\mathbf{q}})}{i\omega_l - \epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}}}.\quad (5.42)$$

The linear response function is simply obtained by $i\omega_l \rightarrow \omega + i\eta$.

5.6 Coulomb interaction and proper and improper response functions

Let us consider the case in which the electron-electron interaction is just the Coulomb repulsion

$$U(\mathbf{q}) = \frac{4\pi e^2}{q^2},$$

which is singular for $q \rightarrow 0$. In order to cure this singularity, it is convenient to recast perturbation theory in a different manner, which naturally brings to identify proper and improper response functions. In Fig. 5.22 we draw the diagrammatic expansion of the density-density correlation function $\chi(\mathbf{q}, i\omega_n)$, which is also the improper response function, up to first order. We can distinguish already two kinds of diagrams: those which can be cut into two by cutting

$$\chi(\mathbf{q}) = \text{(empty loop)} + \text{(loop with one internal line)} + \text{(loop with two external wavy lines)} + \text{(loop with one internal line and one external wavy line)} + \text{(loop with two internal wavy lines)} + \dots$$

Figure 5.22: Diagrammatic expansion of the density-density correlation function up to first order.

an interaction line, as the last diagram, and those which can not, all the others, which we call irreducible with respect to the interaction. Let us define as $\tilde{\chi}(\mathbf{q}, i\omega_n)$ the sum of all irreducible diagrams, in the above sense, whose first order corrections are drawn in Fig. 5.23. We can formally define $\tilde{\chi}(\mathbf{q}, i\omega_n)$ as

$$\tilde{\chi}(\mathbf{q}, i\omega_n) = 2T \sum_m \frac{1}{V} \sum_{\mathbf{k}} G(\mathbf{k} + \mathbf{q}, i\epsilon_m + i\omega_n) G(\mathbf{k}, i\epsilon_m) \tilde{\Lambda}(\mathbf{k} + \mathbf{q}, i\epsilon_m + i\omega_n, \mathbf{k}, i\epsilon_m; \mathbf{q}, i\omega_n), \quad (5.43)$$

by introducing the proper density-vertex function $\tilde{\Lambda}(\mathbf{k}, i\epsilon_m; \mathbf{q}, i\omega_n)$, also shown in the same figure, so to distinguish between Green's function corrections and vertex corrections. Notice that without interaction the density-vertex function is the identity matrix in spin space.

In terms of $\tilde{\chi}(\mathbf{q}, i\omega_n)$ the perturbation expansion of $\chi(\mathbf{q}, i\omega_n)$ can be recast as in the lower panel of Fig. 5.23, which has the formal solution⁴

$$\chi(\mathbf{q}, i\omega_n) = \frac{\tilde{\chi}(\mathbf{q}, i\omega_n)}{1 - \frac{4\pi e^2}{q^2} \tilde{\chi}(\mathbf{q}, i\omega_n)}, \quad (5.44)$$

proving that $\tilde{\chi}(\mathbf{q}, i\omega_n)$ is actually the proper response function.

5.6.1 Screened interaction and corresponding Dyson equation

The proper density-density correlation function allows us to define a screened Coulomb interaction and a dielectric constant through

$$W(\mathbf{q}, i\omega_n) = \frac{4\pi e^2}{q^2 \epsilon(\mathbf{q}, i\omega_n)} = \frac{4\pi e^2}{q^2} \frac{1}{1 - \frac{4\pi e^2}{q^2} \tilde{\chi}(\mathbf{q}, i\omega_n)}, \quad (5.45)$$

The figure consists of three horizontal panels. The top panel shows the proper vertex $\tilde{\chi}(q)$ as a red-shaded loop with a wavy line entering from the left. It is equated to a bare loop plus a series of corrections: a bare loop with a wavy line, a bare loop with a red-shaded loop attached, a bare loop with a red-shaded loop and a wavy line attached, and so on. The middle panel shows the proper density vertex $\tilde{\Lambda}(k+q, k; q)$ as a red-shaded loop with a wavy line entering from the left and a solid line exiting to the right. It is equated to a bare vertex (a dot) plus a series of corrections involving a bare vertex and a red-shaded loop with a wavy line attached. Arrows indicate the flow of momentum $k+q$ and k . The bottom panel shows the improper vertex $\chi(q)$ as a blue-shaded loop. It is equated to the sum of a bare loop and a loop correction involving a red-shaded loop and a blue-shaded loop.

Figure 5.23: Upper panel: The proper $\tilde{\chi}(q)$ up to first order. Middle panel: The proper density-vertex function up to first order. Lower panel: Perturbation expansion of the improper $\chi(\mathbf{q}, i\omega_n)$ in terms of the proper $\tilde{\chi}(q)$.

The figure consists of two horizontal panels. The upper panel shows the screened Coulomb interaction W as a wavy line. It is equated to a bare wavy line plus a loop correction involving a red-shaded loop and a wavy line. The lower panel shows the interaction vertex Γ as a blue-shaded rectangle with a wavy line entering from the left and a solid line exiting to the right. It is equated to the sum of a bare vertex (a dot) and a loop correction involving a red-shaded loop, a wavy line, and another red-shaded loop.

Figure 5.24: Upper panel: Screened Coulomb interaction W . Lower panel: Interaction vertex in terms of the screened interaction and the proper vertex.

which is drawn as a bold wavy line in Fig. 5.24. The interaction vertex Γ which we previously introduced can be also expressed in terms of the screened Coulomb interaction and the proper density-vertex, as also shown in Fig. 5.24. Using this definition for the interaction vertex in the expression of the self-energy, see Fig. 5.19, one finds the alternative definition of the self-energy which is drawn in Fig. 5.25

⁴Notice both the interaction and $\tilde{\chi}(\mathbf{q}, i\omega_n)$, which is a loop, bring a minus sign, hence the sign is plus.

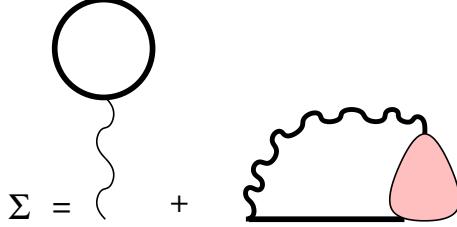


Figure 5.25: Self energy in terms of the screened W and the proper density-vertex.

5.7 Irreducible vertices and the Bethe-Salpeter equations

Let us consider again the interaction vertex (5.40). Let us for instance focus on the upper or the lower incoming and outgoing lines which differ by the momentum/frequency transfer q . This identifies the particle-hole channel at momentum/frequency transfer q . By this definition, we can distinguish two classes of diagrams in the perturbation expansion. The first includes those diagrams which can be divided in two by cutting two fermionic lines within the same particle-hole channel at momentum/frequency q . These type of diagrams are called reducible in the particle-hole channel. For instance the third diagram in Fig. 5.17 belongs to this class. The other class includes all other diagrams which are called irreducible, as the fourth diagram in Fig. 5.17. Let us denote the sum of all irreducible diagrams as

$$\Gamma_{\beta\delta;\gamma\alpha}^0(\mathbf{k} + \mathbf{q} i\epsilon_n + i\omega_l, \mathbf{p} i\epsilon_m; \mathbf{p} + \mathbf{q} i\epsilon_m + i\omega_l, \mathbf{k} i\epsilon_n). \quad (5.46)$$

In terms of Γ^0 the perturbation expansion of Γ can be formally written as

$$\begin{aligned} & \Gamma_{\alpha\beta;\gamma\delta}(\mathbf{k} + \mathbf{q} i\epsilon_n + i\omega_l, \mathbf{p} i\epsilon_m; \mathbf{p} + \mathbf{q} i\epsilon_m + i\omega_l, \mathbf{k} i\epsilon_n) \\ &= \Gamma_{\alpha\beta;\gamma\delta}^0(\mathbf{k} + \mathbf{q} i\epsilon_n + i\omega_l, \mathbf{p} i\epsilon_m; \mathbf{p} + \mathbf{q} i\epsilon_m + i\omega_l, \mathbf{k} i\epsilon_n) \\ &+ \frac{1}{V} \sum_{\mathbf{h}} T \sum_h \sum_{\mu\nu} \Gamma_{\alpha\mu;\nu\delta}^0(\mathbf{k} + \mathbf{q} i\epsilon_n + i\omega_l, \mathbf{h} i\epsilon_h; \mathbf{h} + \mathbf{q} i\epsilon_h + i\omega_l, \mathbf{k} i\epsilon_n) G_\nu(\mathbf{h} + \mathbf{q}, i\epsilon_h + i\omega_l) \\ & G_\mu(\mathbf{h}, i\epsilon_h) \Gamma_{\nu\beta;\mu\delta}(\mathbf{h} + \mathbf{q} i\epsilon_h + i\omega_l, \mathbf{p} i\epsilon_m; \mathbf{p} + \mathbf{q} i\epsilon_m + i\omega_l, \mathbf{h} i\epsilon_h), \end{aligned} \quad (5.47)$$

which is graphically shown in Fig. 5.26. This is the so-called Bathe-Salpeter equation which relates the fully reducible interaction vertex Γ with its irreducible part Γ^0 in the particle-hole channel. Actually, we can proceed in a different way. Namely, instead of selecting the particle-hole channel at momentum transfer q , we can select the two incoming lines, particle-particle channel, which have total momentum/frequency $P = k + p + q$. P is also conserved in the scattering process represented by the interaction vertex. Then we can introduce the concept of reducibility/irreducibility in the particle-particle channel at total momentum/frequency P and identify the irreducible vertex in that channel. Eventually we end up to another Bethe-Salpeter equation, which is shown in Fig. 5.27. In this figure we have denoted the irreducible vertex in

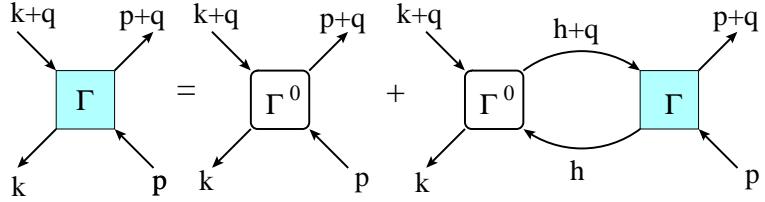


Figure 5.26: Bethe-Salpeter equation for the interaction vertex in the particle-hole channel.

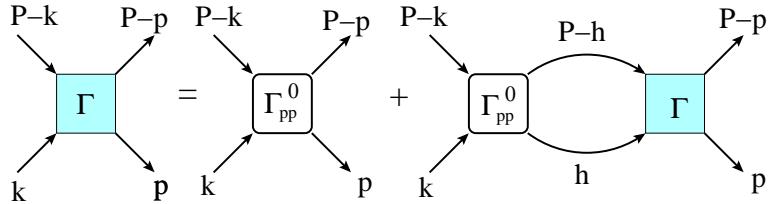


Figure 5.27: Bethe-Salpeter equation for the interaction vertex in the particle-particle channel.

the particle-particle channel as Γ_{pp}^0 to distinguish it from Γ^0 .

5.7.1 Bethe-Salpeter equation for the vertex functions

Let us now introduce the vertex function for a density operator $A(\mathbf{q})$, which is a particle-hole operator, through

$$\langle T_\tau \left(c_{\mathbf{k}\alpha}(\tau_1) c_{\mathbf{k}+\mathbf{q}\beta}^\dagger(\tau_2) A(\mathbf{q}, \tau) \right) \rangle \equiv \int \prod_{i=1}^2 d\tau'_i G_\alpha(\mathbf{k}, \tau_1 - \tau'_1) G_\beta(\mathbf{k} + \mathbf{q}, \tau'_2 - \tau_2) \Lambda_{\alpha\beta}^A(\mathbf{k} \tau'_1, \mathbf{k} + \mathbf{q} \tau'_2; \mathbf{q}, \tau). \quad (5.48)$$

In the absence of interaction, one readily realizes that

$$\Lambda_{\alpha\beta}^A(\mathbf{k} \tau'_1, \mathbf{k} + \mathbf{q} \tau'_2; \mathbf{q}, \tau) = \delta(\tau'_1 - \tau) \delta(\tau'_2 - \tau) \lambda_{\mathbf{k}, \mathbf{k} + \mathbf{q}; \alpha\beta}^A.$$

In the presence of interaction the formal expression of Λ (in what follows we drop the label A) in terms of λ and the interaction vertex can be readily inferred from the expression of the correlation function, and it is graphically shown in Fig. 5.28.

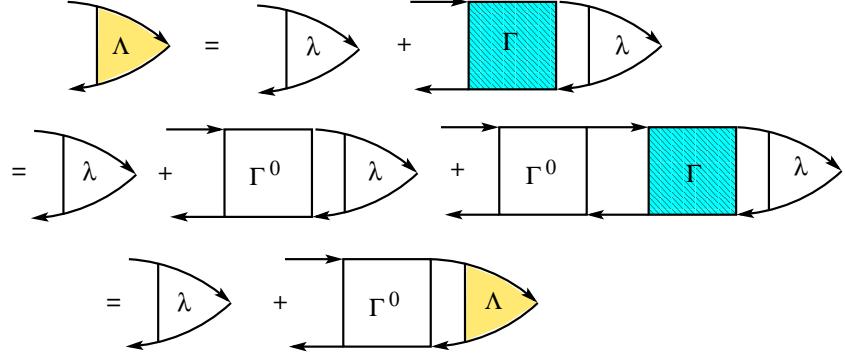


Figure 5.28: Bethe-Salpeter equation for the particle-hole vertex function Λ .

In Fourier space it reads:

$$\begin{aligned} \Lambda_{\alpha\beta}(\mathbf{k} i\epsilon_n, \mathbf{k} + \mathbf{q} i\epsilon_n + i\omega_l; \mathbf{q}, i\omega_l) &= \lambda_{\mathbf{k}, \mathbf{k} + \mathbf{q}; \alpha\beta} \\ &+ \frac{1}{V} \sum_{\mathbf{p}} T \sum_m \sum_{\gamma\delta} \Gamma_{\alpha\gamma; \delta\beta}^0(\mathbf{k} i\epsilon_n, \mathbf{p} + \mathbf{q} i\epsilon_m + i\omega_l; \mathbf{p} i\epsilon_m, \mathbf{k} + \mathbf{q} i\epsilon_n + i\omega_l) \\ G_\gamma(\mathbf{p} + \mathbf{q}, i\epsilon_m + i\omega_l) G_\delta(\mathbf{p}, i\epsilon_m) \Lambda_{\delta\gamma}(\mathbf{p} i\epsilon_m, \mathbf{p} + \mathbf{q} i\epsilon_m + i\omega_l; \mathbf{q}, i\omega_l) \end{aligned} \quad (5.49)$$

$$= \lambda_{\mathbf{k}, \mathbf{k} + \mathbf{q}; \alpha\beta} + \frac{1}{V} \sum_{\mathbf{p}} T \sum_m \sum_{\gamma\delta} \Gamma_{\alpha\gamma; \delta\beta}(\mathbf{k} i\epsilon_n, \mathbf{p} + \mathbf{q} i\epsilon_m + i\omega_l; \mathbf{p} i\epsilon_m, \mathbf{k} + \mathbf{q} i\epsilon_n + i\omega_l)$$

$$G_\gamma(\mathbf{p} + \mathbf{q}, i\epsilon_m + i\omega_l) G_\delta(\mathbf{p}, i\epsilon_m) \lambda_{\mathbf{p}, \mathbf{p} + \mathbf{q}; \delta\gamma}. \quad (5.50)$$

Notice that, in the case of a Coulomb repulsion, the above vertex function for the density operator, i.e. $\lambda_{\mathbf{k}, \mathbf{k} + \mathbf{q}; \alpha\beta}^A = \delta_{\alpha\beta}$, has not to be confused with the proper density-vertex shown in Fig. 5.23. The latter is in fact irreducible with respect to cutting an interaction line, while the former is not. One can easily show that $\tilde{\Lambda}$ satisfies the Bethe-Salpeter equation graphically shown in Fig. 5.29.

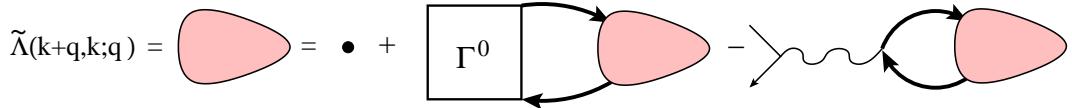


Figure 5.29: Bethe-Salpeter equation for the proper density-vertex function $\tilde{\Lambda}$.

5.8 The Ward identities

Let us suppose that our model has a set of conserved quantities, and let us select one of them, whose density operator we define as

$$J_0(\mathbf{q}) = \sum_{\mathbf{k}} \sum_{ab} c_{\mathbf{k}a}^\dagger \lambda_{\mathbf{k},\mathbf{k}+\mathbf{q};ab}^0 c_{\mathbf{k}+\mathbf{q}b}, \quad (5.51)$$

where to be as general as possible we assume that the roman indices which identify the fermionic operators include both spin as well as other internal labels, like e.g. the band index. We will further assume that the single-particle Green's function are generally non-diagonal in these indices. We can associate to the density operator (5.51) a current density operator $\mathbf{J} = (J_1, J_2, J_3)$ given by

$$\mathbf{J}(\mathbf{q}) = \sum_{\mathbf{k}} \sum_{ab} c_{\mathbf{k}a}^\dagger \lambda_{\mathbf{k},\mathbf{k}+\mathbf{q};ab} c_{\mathbf{k}+\mathbf{q}b}, \quad (5.52)$$

such that the continuity equation in imaginary time is satisfied:

$$\frac{\partial}{\partial \tau} J_0(\mathbf{q}, \tau) + \mathbf{q} \cdot \mathbf{J}(\mathbf{q}, \tau) = 0.$$

If we consider J_0 and \mathbf{J} as the time and space components of a four dimensional current, (J_0, J_1, J_2, J_3) , we can introduce for each component a vertex function through

$$\langle T_\tau \left(c_{\mathbf{k}a}(\tau_1) c_{\mathbf{k}+\mathbf{q}b}^\dagger(\tau_2) J_i(\mathbf{q}, \tau) \right) \rangle.$$

Let us take the time derivative with respect to τ of the zeroth component. The derivative acts either directly on the charge density operator or on the θ -functions which define the time-ordered product. The latter is, dropping for simplicity all indices,

$$\begin{aligned} & [\partial_\tau \theta(\tau_1 - \tau_2) \theta(\tau_2 - \tau)] \langle c(\tau_1) c^\dagger(\tau_2) J_0(\tau) \rangle \\ & + [\partial_\tau \theta(\tau_1 - \tau) \theta(\tau - \tau_2)] \langle c(\tau_1) J_0(\tau) c^\dagger(\tau_2) \rangle \\ & + [\partial_\tau \theta(\tau - \tau_1) \theta(\tau_1 - \tau_2)] \langle J_0(\tau) c(\tau_1) c^\dagger(\tau_2) \rangle \\ & - [\partial_\tau \theta(\tau_2 - \tau_1) \theta(\tau_1 - \tau)] \langle c^\dagger(\tau_2) c(\tau_1) J_0(\tau) \rangle \\ & - [\partial_\tau \theta(\tau_2 - \tau) \theta(\tau - \tau_1)] \langle c^\dagger(\tau_2) J_0(\tau) c(\tau_1) \rangle \\ & - [\partial_\tau \theta(\tau - \tau_2) \theta(\tau_2 - \tau_1)] \langle J_0(\tau) c^\dagger(\tau_2) c(\tau_1) \rangle \\ &= -\theta(\tau_1 - \tau_2) \delta(\tau_2 - \tau) \langle c(\tau_1) c^\dagger(\tau_2) J_0(\tau) \rangle \\ & + [-\delta(\tau_1 - \tau) \theta(\tau - \tau_2) + \theta(\tau_1 - \tau) \delta(\tau - \tau_2)] \langle c(\tau_1) J_0(\tau) c^\dagger(\tau_2) \rangle \\ & + \delta(\tau - \tau_1) \theta(\tau_1 - \tau_2) \langle J_0(\tau) c(\tau_1) c^\dagger(\tau_2) \rangle \\ & + \theta(\tau_2 - \tau_1) \delta(\tau_1 - \tau) \langle c^\dagger(\tau_2) c(\tau_1) J_0(\tau) \rangle \\ & - [-\delta(\tau_2 - \tau) \theta(\tau - \tau_1) + \theta(\tau_2 - \tau) \delta(\tau - \tau_1)] \langle c^\dagger(\tau_2) J_0(\tau) c(\tau_1) \rangle \end{aligned}$$

$$\begin{aligned}
& -\delta(\tau - \tau_2)\theta(\tau_2 - \tau_1) \langle J_0(\tau) c^\dagger(\tau_2) c(\tau_1) \rangle \\
= & \delta(\tau - \tau_2) \langle T_\tau \left(c(\tau_1) [J_0(\tau), c^\dagger(\tau)] \right) \rangle \\
& + \delta(\tau - \tau_1) \langle T_\tau \left([J_0(\tau), c(\tau)] c^\dagger(\tau_2) \right) \rangle.
\end{aligned}$$

It can be readily shown that

$$\begin{aligned}
\sum_{\mathbf{p}} \sum_{cd} \left[c_{\mathbf{p}c}^\dagger \lambda_{\mathbf{p},\mathbf{p}+\mathbf{q};cd}^0 c_{\mathbf{p}+\mathbf{q}d}, c_{\mathbf{k}+\mathbf{q}b}^\dagger \right] &= \sum_c c_{\mathbf{k}c}^\dagger \lambda_{\mathbf{k},\mathbf{k}+\mathbf{q};cb}^0 \\
\sum_{\mathbf{p}} \sum_{cd} \left[c_{\mathbf{p}c}^\dagger \lambda_{\mathbf{p},\mathbf{p}+\mathbf{q};cd}^0 c_{\mathbf{p}+\mathbf{q}d}, c_{\mathbf{k}a} \right] &= - \sum_d \lambda_{\mathbf{k},\mathbf{k}+\mathbf{q};ad}^0 c_{\mathbf{k}+\mathbf{q}d},
\end{aligned}$$

so that the above time-derivative becomes

$$\begin{aligned}
& \sum_c \delta(\tau - \tau_2) \langle T_\tau \left(c_{\mathbf{k}a}(\tau_1) c_{\mathbf{k}c}^\dagger(\tau) \lambda_{\mathbf{k},\mathbf{k}+\mathbf{q};cb}^0 \right) \rangle \\
& - \sum_d \delta(\tau - \tau_1) \langle T_\tau \left(\lambda_{\mathbf{k},\mathbf{k}+\mathbf{q};ad}^0 c_{\mathbf{k}+\mathbf{q}d}(\tau) c_{\mathbf{k}+\mathbf{q}b}^\dagger(\tau_2) \right) \rangle \\
= & - \sum_c \delta(\tau - \tau_2) G_{ac}(\mathbf{k}, \tau_1 - \tau) \lambda_{\mathbf{k},\mathbf{k}+\mathbf{q};cb}^0 \\
& + \sum_d \delta(\tau - \tau_1) \lambda_{\mathbf{k},\mathbf{k}+\mathbf{q};ad}^0 G_{db}(\mathbf{k} + \mathbf{q}, \tau - \tau_2).
\end{aligned}$$

In conclusion we find, making use of the continuity equation,

$$\begin{aligned}
& \frac{\partial}{\partial \tau} \langle T_\tau \left(c_{\mathbf{k}a}(\tau_1) c_{\mathbf{k}+\mathbf{q}b}^\dagger(\tau_2) J_0(\mathbf{q}, \tau) \right) \rangle = \langle T_\tau \left(c_{\mathbf{k}a}(\tau_1) c_{\mathbf{k}+\mathbf{q}b}^\dagger(\tau_2) \frac{\partial J_0(\mathbf{q}, \tau)}{\partial \tau} \right) \rangle \\
& - \sum_c \delta(\tau - \tau_2) G_{ac}(\mathbf{k}, \tau_1 - \tau) \lambda_{\mathbf{k},\mathbf{k}+\mathbf{q};cb}^0 \\
& + \sum_d \delta(\tau - \tau_1) \lambda_{\mathbf{k},\mathbf{k}+\mathbf{q};ad}^0 G_{db}(\mathbf{k} + \mathbf{q}, \tau - \tau_2) \\
= & - \langle T_\tau \left(c_{\mathbf{k}a}(\tau_1) c_{\mathbf{k}+\mathbf{q}b}^\dagger(\tau_2) \mathbf{q} \cdot \mathbf{J}(\mathbf{q}, \tau) \right) \rangle \\
& - \sum_c \delta(\tau - \tau_2) G_{ac}(\mathbf{k}, \tau_1 - \tau) \lambda_{\mathbf{k},\mathbf{k}+\mathbf{q};cb}^0 \\
& + \sum_d \delta(\tau - \tau_1) \lambda_{\mathbf{k},\mathbf{k}+\mathbf{q};ad}^0 G_{db}(\mathbf{k} + \mathbf{q}, \tau - \tau_2).
\end{aligned}$$

Upon introducing the vertex functions for the charge and current densities, Λ^0 and $\mathbf{\Lambda}$, respectively, and Fourier transforming in frequency we find

$$\sum_{cd} G_{ac}(\mathbf{k}, i\epsilon_n) G_{db}(\mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l)$$

$$\begin{aligned} & \left(-i\omega_l \Lambda_{cd}^0(\mathbf{k}, i\epsilon_n, \mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l; \mathbf{q}, i\omega_l) + \mathbf{q} \cdot \boldsymbol{\Lambda}_{cd}(\mathbf{k}, i\epsilon_n, \mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l; \mathbf{q}, i\omega_l) \right) \\ & = - \sum_c G_{ac}(\mathbf{k}, i\epsilon_n) \lambda_{\mathbf{k}, \mathbf{k} + \mathbf{q}; cb}^0 + \sum_d \lambda_{\mathbf{k}, \mathbf{k} + \mathbf{q}; ad}^0 G_{db}(\mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l). \end{aligned} \quad (5.53)$$

By means of the Bethe-Salpeter equation for the vertex functions (5.49) we can rewrite this equation as

$$\begin{aligned} & \sum_{cd} G_{ac}(\mathbf{k}, i\epsilon_n) G_{db}(\mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l) \\ & \left(-i\omega_l \Lambda_{cd}^0(\mathbf{k}, i\epsilon_n, \mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l; \mathbf{q}, i\omega_l) + \mathbf{q} \cdot \boldsymbol{\Lambda}_{cd}(\mathbf{k}, i\epsilon_n, \mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l; \mathbf{q}, i\omega_l) \right) \\ & = \sum_{cd} G_{ac}(\mathbf{k}, i\epsilon_n) G_{db}(\mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l) \left(-i\omega_l \lambda_{\mathbf{k}, \mathbf{k} + \mathbf{q}; cd}^0 + \mathbf{q} \cdot \boldsymbol{\lambda}_{\mathbf{k}, \mathbf{k} + \mathbf{q}; cd} \right) \\ & \quad + \frac{1}{V} \sum_{\mathbf{p}} T \sum_m \sum_{cdefgh} G_{ac}(\mathbf{k}, i\epsilon_n) G_{db}(\mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l) \\ & \quad \Gamma_{ce; fd}^0(\mathbf{k}, i\epsilon_n, \mathbf{p} + \mathbf{q}, i\epsilon_m + i\omega_l; \mathbf{p}, i\epsilon_m, \mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l) \\ & \quad G_{fg}(\mathbf{p}, i\epsilon_m) G_{he}(\mathbf{p} + \mathbf{q}, i\epsilon_m + i\omega_l) \\ & \quad \left(-i\omega_l \Lambda_{gh}^0(\mathbf{p}, i\epsilon_m, \mathbf{p} + \mathbf{q}, i\epsilon_m + i\omega_l; \mathbf{q}, i\omega_l) + \mathbf{q} \cdot \boldsymbol{\Lambda}_{gh}(\mathbf{p}, i\epsilon_m, \mathbf{p} + \mathbf{q}, i\epsilon_m + i\omega_l; \mathbf{q}, i\omega_l) \right) \\ & = - \sum_c G_{ac}(\mathbf{k}, i\epsilon_n) \lambda_{\mathbf{k}, \mathbf{k} + \mathbf{q}; cb}^0 + \sum_d \lambda_{\mathbf{k}, \mathbf{k} + \mathbf{q}; ad}^0 G_{db}(\mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l) \\ & = \sum_{cd} G_{ac}(\mathbf{k}, i\epsilon_n) G_{db}(\mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l) \left(-i\omega_l \lambda_{\mathbf{k}, \mathbf{k} + \mathbf{q}; cd}^0 + \mathbf{q} \cdot \boldsymbol{\lambda}_{\mathbf{k}, \mathbf{k} + \mathbf{q}; cd} \right) \\ & \quad + \frac{1}{V} \sum_{\mathbf{p}} T \sum_m \sum_{cdef} G_{ac}(\mathbf{k}, i\epsilon_n) G_{db}(\mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l) \\ & \quad \Gamma_{ce; fd}^0(\mathbf{k}, i\epsilon_n, \mathbf{p} + \mathbf{q}, i\epsilon_m + i\omega_l; \mathbf{p}, i\epsilon_m, \mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l) \\ & \quad \left(- \sum_g G_{fg}(\mathbf{p}, i\epsilon_m) \lambda_{\mathbf{p}, \mathbf{p} + \mathbf{q}; ge}^0 + \sum_h \lambda_{\mathbf{p}, \mathbf{p} + \mathbf{q}; fh}^0 G_{he}(\mathbf{p} + \mathbf{q}, i\epsilon_m + i\omega_l) \right). \end{aligned}$$

If we multiply both sides by the matrix product $\hat{G}^{-1}(\mathbf{k}, i\epsilon_n) \hat{G}^{-1}(\mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l)$ ⁵, we get

$$\begin{aligned} & \left(-i\omega_l \Lambda_{ab}^0(\mathbf{k}, i\epsilon_n, \mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l; \mathbf{q}, i\omega_l) + \mathbf{q} \cdot \boldsymbol{\Lambda}_{ab}(\mathbf{k}, i\epsilon_n, \mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l; \mathbf{q}, i\omega_l) \right) \\ & = \left(-i\omega_l \lambda_{\mathbf{k}, \mathbf{k} + \mathbf{q}; ab}^0 + \mathbf{q} \cdot \boldsymbol{\lambda}_{\mathbf{k}, \mathbf{k} + \mathbf{q}; ab} \right) \\ & \quad + \frac{1}{V} \sum_{\mathbf{p}} T \sum_m \sum_{ef} \Gamma_{ae; fb}^0(\mathbf{k}, i\epsilon_n, \mathbf{p} + \mathbf{q}, i\epsilon_m + i\omega_l; \mathbf{p}, i\epsilon_m, \mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l) \end{aligned}$$

⁵The Green's function G_{ab} can be interpreted as the ab component of a matrix \hat{G}

$$\begin{aligned} & \left(- \sum_g G_{fg}(\mathbf{p}, i\epsilon_m) \lambda_{\mathbf{p}, \mathbf{p}+\mathbf{q}; ge}^0 + \sum_h \lambda_{\mathbf{p}, \mathbf{p}+\mathbf{q}; fh}^0 G_{he}(\mathbf{p} + \mathbf{q}, i\epsilon_m + i\omega_l) \right) \\ &= - \sum_d \lambda_{\mathbf{k}, \mathbf{k}+\mathbf{q}; ad}^0 G_{db}^{-1}(\mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l) + \sum_c G_{ac}^{-1}(\mathbf{k}, i\epsilon_n) \lambda_{\mathbf{k}, \mathbf{k}+\mathbf{q}; cb}^0. \end{aligned}$$

We notice that the non-interacting Green's functions satisfy the same equation with $\Gamma^0 = 0$, namely

$$\begin{aligned} & \left(-i\omega_l \lambda_{\mathbf{k}, \mathbf{k}+\mathbf{q}; ab}^0 + \mathbf{q} \cdot \boldsymbol{\lambda}_{\mathbf{k}, \mathbf{k}+\mathbf{q}; ab} \right) = - \sum_d \lambda_{\mathbf{k}, \mathbf{k}+\mathbf{q}; ad}^0 \left(G^{(0)} \right)_{db}^{-1}(\mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l) \\ &+ \sum_c \left(G^{(0)} \right)_{ac}^{-1}(\mathbf{k}, i\epsilon_n) \lambda_{\mathbf{k}, \mathbf{k}+\mathbf{q}; cb}^0, \end{aligned}$$

so that we can write

$$\begin{aligned} & \frac{1}{V} \sum_{\mathbf{p}} T \sum_m \sum_{ef} \Gamma_{ae; fb}^0(\mathbf{k} i\epsilon_n, \mathbf{p} + \mathbf{q} i\epsilon_m + i\omega_l; \mathbf{p} i\epsilon_m, \mathbf{k} + \mathbf{q} i\epsilon_n + i\omega_l) \\ & \left(- \sum_g G_{fg}(\mathbf{p}, i\epsilon_m) \lambda_{\mathbf{p}, \mathbf{p}+\mathbf{q}; ge}^0 + \sum_h \lambda_{\mathbf{p}, \mathbf{p}+\mathbf{q}; fh}^0 G_{he}(\mathbf{p} + \mathbf{q}, i\epsilon_m + i\omega_l) \right) \\ &= - \sum_d \lambda_{\mathbf{k}, \mathbf{k}+\mathbf{q}; ad}^0 \left(G_{db}^{-1}(\mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l) - \left(G^{(0)} \right)_{db}^{-1}(\mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l) \right) \\ &+ \sum_c \left(G_{ac}^{-1}(\mathbf{k}, i\epsilon_n) - \left(G^{(0)} \right)_{ac}^{-1}(\mathbf{k}, i\epsilon_n) \right) \lambda_{\mathbf{k}, \mathbf{k}+\mathbf{q}; cb}^0. \end{aligned}$$

By definition

$$\hat{G}^{-1} - \left(\hat{G}^{(0)} \right)^{-1} = -\hat{\Sigma},$$

where $\hat{\Sigma}$ is the self-energy matrix, so that

$$\begin{aligned} & \sum_c \lambda_{\mathbf{k}, \mathbf{k}+\mathbf{q}; ac}^0 \Sigma_{cb}(\mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l) - \Sigma_{ac}(\mathbf{k}, i\epsilon_n) \lambda_{\mathbf{k}, \mathbf{k}+\mathbf{q}; cb}^0 \\ &= \frac{1}{V} \sum_{\mathbf{p}} T \sum_m \sum_{cd} \Gamma_{ac; db}^0(\mathbf{k} i\epsilon_n, \mathbf{p} + \mathbf{q} i\epsilon_m + i\omega_l; \mathbf{p} i\epsilon_m, \mathbf{k} + \mathbf{q} i\epsilon_n + i\omega_l) \\ & \sum_e \left(-G_{de}(\mathbf{p}, i\epsilon_m) \lambda_{\mathbf{p}, \mathbf{p}+\mathbf{q}; ec}^0 + \lambda_{\mathbf{p}, \mathbf{p}+\mathbf{q}; de}^0 G_{ec}(\mathbf{p} + \mathbf{q}, i\epsilon_m + i\omega_l) \right). \end{aligned} \tag{5.54}$$

This is the so-called Ward identity which is a consequence of conservation laws. There are other two equivalent ways to rewrite this identity. Indeed, through (5.53), we can also write

$$\begin{aligned} & \sum_c \lambda_{\mathbf{k}, \mathbf{k}+\mathbf{q}; ac}^0 \Sigma_{cb}(\mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l) - \Sigma_{ac}(\mathbf{k}, i\epsilon_n) \lambda_{\mathbf{k}, \mathbf{k}+\mathbf{q}; cb}^0 \\ &= \frac{1}{V} \sum_{\mathbf{p}} T \sum_m \sum_{cd} \Gamma_{ac; db}^0(\mathbf{k} i\epsilon_n, \mathbf{p} + \mathbf{q} i\epsilon_m + i\omega_l; \mathbf{p} i\epsilon_m, \mathbf{k} + \mathbf{q} i\epsilon_n + i\omega_l) \\ & \quad G_{de}(\mathbf{p}, i\epsilon_m) G_{fc}(\mathbf{p} + \mathbf{q}, i\epsilon_m + i\omega_l) \\ & \quad \left(-i\omega_l \Lambda_{ef}^0(\mathbf{p} i\epsilon_m, \mathbf{p} + \mathbf{q} i\epsilon_m + i\omega_l; \mathbf{q} i\omega_l) + \mathbf{q} \cdot \boldsymbol{\Lambda}_{ef}(\mathbf{p} i\epsilon_m, \mathbf{p} + \mathbf{q} i\epsilon_m + i\omega_l; \mathbf{q} i\omega_l) \right). \end{aligned} \quad (5.55)$$

Furthermore, using the fully reducible vertex Γ instead of Γ^0 , see Eq. (5.50), we also find

$$\begin{aligned} & \sum_c \lambda_{\mathbf{k}, \mathbf{k}+\mathbf{q}; ac}^0 \Sigma_{cb}(\mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l) - \Sigma_{ac}(\mathbf{k}, i\epsilon_n) \lambda_{\mathbf{k}, \mathbf{k}+\mathbf{q}; cb}^0 \\ &= \frac{1}{V} \sum_{\mathbf{p}} T \sum_m \sum_{cd} \Gamma_{ac; db}(\mathbf{k} i\epsilon_n, \mathbf{p} + \mathbf{q} i\epsilon_m + i\omega_l; \mathbf{p} i\epsilon_m, \mathbf{k} + \mathbf{q} i\epsilon_n + i\omega_l) \\ & \quad G_{de}(\mathbf{p}, i\epsilon_m) G_{fc}(\mathbf{p} + \mathbf{q}, i\epsilon_m + i\omega_l) \left(-i\omega_l \lambda_{\mathbf{p}, \mathbf{p}+\mathbf{q}; ef}^0 + \mathbf{q} \cdot \boldsymbol{\lambda}_{\mathbf{p}, \mathbf{p}+\mathbf{q}; ef} \right). \end{aligned} \quad (5.56)$$

5.9 Consistent approximation schemes

Since it is usually impossible to sum up all orders in perturbation theory, one is forced to make some approximation on the self-energy. In doing that, one would like not to spoil any conservation law. In this section we show what is the proper way to define an approximation scheme which is consistent with the conservation laws.

In general we can recast the perturbation expansion for the self-energy in terms of the fully interacting Green's functions instead of the non-interacting ones. This kind of expansion is called skeleton expansion, the diagrams up to second order being drawn in Fig. 5.30. This allows us

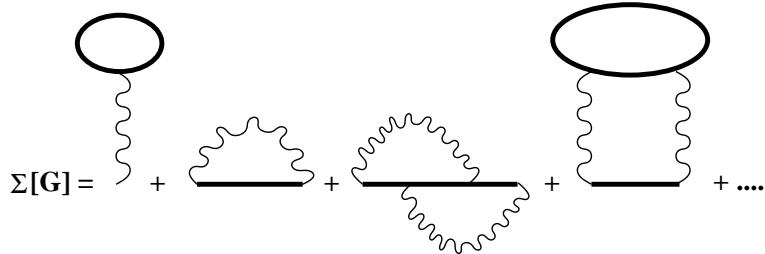


Figure 5.30: Skeleton expansion for the self-energy up to second order in the interaction.

to assume formally that the self-energy is a functional of the Green's function $\Sigma[G]$. Let us

calculate the functional derivative of Σ with respect to G . Let us imagine to do it graphically, as shown in Fig. 5.31. Namely, we take out of the rounded box, which represents the whole

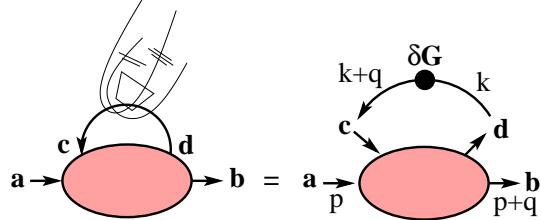


Figure 5.31: Graphical representation of $\delta\Sigma/\delta G$.

skeleton expansion of Σ , a Green's function G and we vary it, δG . Therefore $\delta\Sigma/\delta G$ is a four leg vertex. What can it be? One easily realizes that, since the functional derivative is done with respect to the fully interacting Green's function, this four leg vertex is just the irreducible Γ^0 in the particle-hole channel. Therefore

$$\frac{\delta\Sigma_{ab}(p, p+q)}{\delta G_{dc}(k, k+q)} = \Gamma_{ac;db}^0(p, k+q; k, p+q). \quad (5.57)$$

We further notice that

$$\delta G_{dc}(k, k+q) = - \sum_{ef} G_{de}(k) \left[\delta \left(G_{ef}^{(0)}(k, k+q) \right)^{-1} - \delta\Sigma_{ef}(k, k+q) \right] G_{fc}(k+q),$$

which inserted into (5.57) and solving for $\delta\Sigma$ leads to

$$\begin{aligned} \delta\Sigma_{ab}(p, p+q) &= \int dk \Gamma_{ac;db}^0(p, k+q; k, p+q) \delta G_{dc}(k, k+q) \\ &= - \sum_{ef} \int dk \Gamma_{ac;db}(p, k+q; k, p+q) G_{de}(k) \delta G_{ef}^{(0)}(k, k+q)^{-1} G_{fc}(k+q), \end{aligned} \quad (5.58)$$

where we used the Bethe-Salpeter equation for Γ versus Γ^0 .

We notice that (5.57) is perfectly consistent with the Ward identity (5.54). Since the Ward identities are consequence of conservation laws, we get to the following conclusion:

If the self-energy is approximated with a functional $\Sigma_{appx}[G]$, this approximation is consistent with the conservation laws if the irreducible vertex is also approximated by

$$\Gamma_{appx}^0 = \frac{\delta\Sigma_{appx}[G]}{\delta G}.$$

Finally we notice that, given an approximate $\Sigma_{appx}[G]$, then the actual Green's function is obtained by solving the self-consistency equation:

$$G^{-1} = \left(G^{(0)} \right)^{-1} - \Sigma_{appx}[G]. \quad (5.59)$$

5.9.1 Example: the Hartree-Fock approximation

Let us consider the interacting Hamiltonian

$$H = \sum_{ab} t_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{abcd} U_{acdb} c_a^\dagger c_c^\dagger c_d c_b.$$

Let us approximate the skeleton expansion of the self-energy with the two first-order diagrams, as shown in Fig. 5.32. This amounts to the following expression of the self-energy

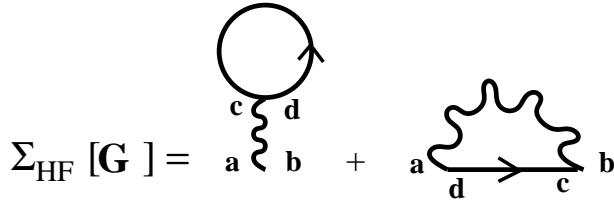


Figure 5.32: Skeleton expansion in the Hartree-Fock approximation.

$$\Sigma_{ab}(i\epsilon_n) = T \sum_m \sum_{cd} U_{acdb} e^{-i\epsilon_m 0^-} G_{dc}(i\epsilon_m) - T \sum_m \sum_{cd} U_{acbd} e^{-i\epsilon_m 0^-} G_{dc}(i\epsilon_m). \quad (5.60)$$

We notice that

$$T \sum_m e^{-i\epsilon_m 0^-} G_{dc}(i\epsilon_m) = G_{dc}(\tau = 0^-) = \langle c_c^\dagger c_d \rangle \equiv \Delta_{cd}.$$

The Green's function satisfies the self-consistency equation (5.59), which in this case reads

$$(G^{-1})_{ab} = i\epsilon_n - t_{ab} - \Sigma_{ab} = i\epsilon_n - t_{ab} - \sum_{cd} \Delta_{cd} (U_{acdb} - U_{acbd}),$$

which is diagonalized by diagonalizing

$$t_{ab} + \sum_{cd} \Delta_{cd} (U_{acdb} - U_{acbd}) = (H_{HF})_{ab},$$

which is nothing but the Hartree-Fock Hamiltonian. Namely, the self-consistency requirement (5.59) is just the Hartree-Fock self-consistency equation.

In order to have a consistent scheme, we need to approximate Γ^0 as

$$\Gamma_{acdb}^0 = \frac{\delta \Sigma_{ab}}{\delta G_{dc}} = U_{acdb} - U_{acbd}.$$

One can readily show that the correlation functions calculated with the above Γ^0 coincide with the time-dependent Hartree-Fock, which is therefore a consistent approximation.

5.10 Some additional properties and useful results

In this final section we derive some properties that may be useful in several contexts.

5.10.1 The occupation number and the Luttinger-Ward functional

By the definition of the single-particle Green's function in momentum space, one can derive the average values

$$\Delta_{\mathbf{k}ab} = \langle c_{\mathbf{kb}}^\dagger c_{\mathbf{ka}} \rangle,$$

where the labels a and b include spin and additional internal indices, through

$$\begin{aligned}\hat{\Delta}_{\mathbf{k}} &= \hat{G}(\mathbf{k}, \tau = 0^-) = T \sum_n \hat{G}(\mathbf{k}, i\epsilon_n) e^{-i\epsilon_n 0^-} \\ &= T \sum_n \frac{1}{i\epsilon_n - \hat{\epsilon}_{\mathbf{k}} - \hat{\Sigma}(\mathbf{k}, i\epsilon_n)} e^{-i\epsilon_n 0^-},\end{aligned}$$

where $\hat{\Delta}_{\mathbf{k}}$, $\hat{\epsilon}_{\mathbf{k}}$ and $\hat{\Sigma}(\mathbf{k}, i\epsilon_n)$ are matrices in the a -space. We define $\epsilon_0 = \pi T$ such that, for $T \rightarrow 0$, $\epsilon_0 \rightarrow 0$, which allows to formally introduce the derivative with respect to the Matsubara frequencies. One finds that

$$\begin{aligned}\hat{G}(\mathbf{k}, i\epsilon_n) &= \frac{1}{i\epsilon_n - \hat{\epsilon}_{\mathbf{k}} - \hat{\Sigma}(\mathbf{k}, i\epsilon_n)} \\ &= \frac{\ln \hat{G}^{-1}(\mathbf{k}, i\epsilon_n + i\epsilon_0) - \ln \hat{G}^{-1}(\mathbf{k}, i\epsilon_n)}{i\epsilon_0} + \hat{G}(\mathbf{k}, i\epsilon_n) \frac{\hat{\Sigma}(\mathbf{k}, i\epsilon_n + i\epsilon_0) - \hat{\Sigma}(\mathbf{k}, i\epsilon_n)}{i\epsilon_0} \\ &= \frac{\partial \ln \hat{G}^{-1}(\mathbf{k}, i\epsilon_n)}{\partial i\epsilon_n} + \hat{G}(\mathbf{k}, i\epsilon_n) \frac{\partial \hat{\Sigma}(\mathbf{k}, i\epsilon_n)}{\partial i\epsilon_n},\end{aligned}$$

hence

$$\hat{\Delta}_{\mathbf{k}} = T \sum_n \left(\frac{\partial \ln \hat{G}_\sigma^{-1}(\mathbf{k}, i\epsilon_n)}{\partial i\epsilon_n} + \hat{G}(\mathbf{k}, i\epsilon_n) \frac{\partial \hat{\Sigma}(\mathbf{k}, i\epsilon_n)}{\partial i\epsilon_n} \right) e^{-i\epsilon_n 0^-}. \quad (5.61)$$

Let us concentrate on the second term in (5.61). By the definition of the derivatives it follows that

$$T \sum_n \hat{G}(\mathbf{k}, i\epsilon_n) \frac{\partial \hat{\Sigma}(\mathbf{k}, i\epsilon_n)}{\partial i\epsilon_n} = -T \sum_n \frac{\partial \hat{G}(\mathbf{k}, i\epsilon_n)}{\partial i\epsilon_n} \hat{\Sigma}(\mathbf{k}, i\epsilon_n).$$

The interacting Hamiltonian allows for several conserved quantities. Let us write a generic one of them like

$$\mathcal{M} = \sum_{\mathbf{k}} \sum_{ab} c_{\mathbf{ka}}^\dagger M_{ab}(\mathbf{k}) c_{\mathbf{kb}}.$$

It turns out that the average value of \mathcal{M} is given by

$$\langle \mathcal{M} \rangle = \sum_{\mathbf{k}} m_{\mathbf{k}},$$

where

$$\begin{aligned} m_{\mathbf{k}} &= \text{Tr}\left(M(\mathbf{k}) \Delta_{\mathbf{k}}\right) = T \sum_n \left[\text{Tr}\left(M(\mathbf{k}) \frac{\partial \ln \hat{G}^{-1}(\mathbf{k}, i\epsilon_n)}{\partial i\epsilon_n}\right) \right. \\ &\quad \left. - \text{Tr}\left(M(\mathbf{k}) \frac{\partial \hat{G}(\mathbf{k}, i\epsilon_n)}{\partial i\epsilon_n} \hat{\Sigma}(\mathbf{k}, i\epsilon_n)\right) e^{-i\epsilon_n 0^-} \right]. \end{aligned}$$

We draw in Fig. 5.33 the first orders in the skeleton expansion of the functional of the fully-interacting Green's function $X[G]$, introduced originally by Luttinger and Ward. It is obtained from the skeleton expansion of the self-energy by connecting the external vertices with a fully-interacting Green's function and dividing each term by $1/2n$, where $2n$ is the number of Green's functions, n being the number of interaction lines.⁶ By its definition, one can readily verify

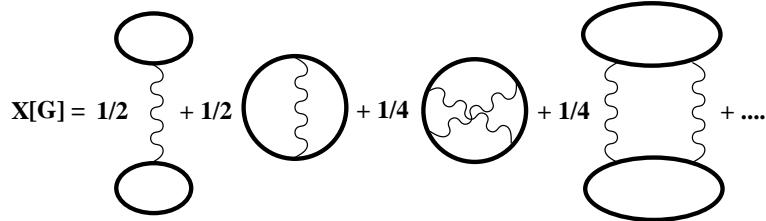


Figure 5.33: Graphical representation of the functional $X[G]$.

that $X[G]$ satisfies

$$\delta X[G(\mathbf{k})] = T \sum_n \text{Tr}\left(\hat{\Sigma}(\mathbf{k}, i\epsilon_n) \delta \hat{G}(\mathbf{k}, i\epsilon_n)\right), \quad (5.62)$$

namely the self-energy is the functional derivative of X . One can readily show that, for any

⁶The self-energy itself is a functional of G , which guarantees that X is a well defined functional.

conserved quantity, the following result holds:⁷

$$\delta X[G(\mathbf{k})] = T \sum_n \text{Tr} \left[\hat{\Sigma}(\mathbf{k}, i\epsilon_n) M(\mathbf{k}) \frac{\partial \hat{G}(\mathbf{k}, i\epsilon_n)}{\partial i\epsilon_0} \right] \delta i\epsilon_0 = 0. \quad (5.63)$$

⁷To prove Eq. (5.63), let us assume to rotate the basis into the one in which the hermitean matrix $\hat{M}(\mathbf{k})$ is diagonal, with eigenvalues $m_\alpha(\mathbf{k})$. The fermion operators in the new basis are accordingly $c_{\mathbf{k}\alpha}$ and $c_{\mathbf{k}\alpha}^\dagger$, hence the conserved operator becomes

$$\mathcal{M} = \sum_{\mathbf{k}\alpha} m_\alpha(\mathbf{k}) c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}\alpha}.$$

The fully interacting Green's function must be diagonal in α for \mathcal{M} to commute with the Hamiltonian

$$0 = [\mathcal{H}, \mathcal{M}] = [\mathcal{H}_0, \mathcal{M}] + [\mathcal{H}_{int}, \mathcal{M}].$$

Note that, because the first commutator is a one-body operator while the second a two-body one, it follows that

$$[\mathcal{H}_0, \mathcal{M}] = 0, \quad [\mathcal{H}_{int}, \mathcal{M}] = 0.$$

Now suppose that, within the perturbative calculation of the Luttinger-Ward functional X , which just amounts to calculate the average value of products of $\mathcal{H}_{int}(\tau)$ in the interaction representation at different times, each interaction vertex

$$\mathcal{H}_{int}(\tau) = e^{\mathcal{H}_0\tau} \mathcal{H}_{int} e^{-\mathcal{H}_0\tau},$$

is transformed into

$$\mathcal{H}'_{int}(\tau) = e^{i\epsilon_0 \mathcal{M}\tau} e^{\mathcal{H}_0\tau} \mathcal{H}_{int} e^{-\mathcal{H}_0\tau} e^{-i\epsilon_0 \mathcal{M}\tau},$$

where $\epsilon_0 = \pi T$. Since \mathcal{H}_{int} and \mathcal{H}_0 commute separately with \mathcal{M} , it follows that $\mathcal{H}'_{int}(\tau) = \mathcal{H}_{int}(\tau)$; indeed

$$\begin{aligned} \mathcal{H}'_{int}(\tau) &= e^{i\epsilon_0 \mathcal{M}\tau} e^{\mathcal{H}_0\tau} \mathcal{H}_{int} e^{-\mathcal{H}_0\tau} e^{-i\epsilon_0 \mathcal{M}\tau} \\ &= e^{\mathcal{H}_0\tau} e^{i\epsilon_0 \mathcal{M}\tau} \mathcal{H}_{int} e^{-i\epsilon_0 \mathcal{M}\tau} e^{-\mathcal{H}_0\tau} \\ &= e^{\mathcal{H}_0\tau} \mathcal{H}_{int} e^{-\mathcal{H}_0\tau} = \mathcal{H}_{int}(\tau). \end{aligned}$$

Therefore the Luttinger-Ward functional X is invariant to this transformation. On the other hand, instead of transforming the interaction as a whole, I can also transform each fermionic operator inside the interaction separately, that implies, in the Heisenberg representation,

$$\begin{aligned} c_{\mathbf{k}\alpha}(\tau) &= e^{\mathcal{H}\tau} c_{\mathbf{k}\alpha} e^{-\mathcal{H}\tau} \rightarrow e^{i\epsilon_0 \mathcal{M}\tau} c_{\mathbf{k}\alpha}(\tau) e^{-i\epsilon_0 \mathcal{M}\tau} \\ &= e^{-i\epsilon_0 m_\alpha(\mathbf{k})\tau} c_{\mathbf{k}\alpha}(\tau), \end{aligned}$$

and accordingly that the Green's function changes into

$$G_\alpha(\mathbf{k}, \tau - \tau') \rightarrow e^{-i\epsilon_0 m_\alpha(\mathbf{k})(\tau - \tau')} G_\alpha(\mathbf{k}, \tau - \tau'),$$

namely

$$G_\alpha(\mathbf{k}, i\epsilon_n) \rightarrow G_\alpha(\mathbf{k}, i\epsilon_n + i\epsilon_0 m_\alpha(\mathbf{k})).$$

Since the final result must not change, we get to the conclusion that

$$\begin{aligned} \delta X[G] &= X[G_\alpha(\mathbf{k}, i\epsilon_n + i\epsilon_0 m_\alpha(\mathbf{k}))] - X[G_\alpha(\mathbf{k}, i\epsilon_n)] \\ &= T \sum_n \sum_\alpha \Sigma_\alpha(\mathbf{k}, i\epsilon_n) m_\alpha(\mathbf{k}) \frac{\partial G_\alpha(\mathbf{k}, i\epsilon_n)}{\partial i\epsilon_0} \delta i\epsilon_0 = 0. \end{aligned}$$

After back-rotation in the original basis, we recover Eq. (5.63).

As a result we obtain that

$$m_{\mathbf{k}} = T \sum_n \text{Tr} \left(M(\mathbf{k}) \frac{\partial \ln \hat{G}^{-1}(\mathbf{k}, i\epsilon_n)}{\partial i\epsilon_n} \right) e^{-i\epsilon_n 0^-}. \quad (5.64)$$

We already showed that the Green's function, hence also its logarithm, has generally branch cuts on the real axis. By means of (5.9) we then find⁸

$$\begin{aligned} m_{\mathbf{k}} &= T \sum_n \text{Tr} \left(M(\mathbf{k}) \frac{\partial \ln \hat{G}^{-1}(\mathbf{k}, i\epsilon_n)}{\partial i\epsilon_n} \right) e^{-i\epsilon_n 0^-} \\ &= - \int \frac{d\epsilon}{\pi} f(\epsilon) \frac{\partial}{\partial \epsilon} \text{Arg} \text{Tr} \left(M(\mathbf{k}) \ln \hat{G}^{-1}(\mathbf{k}, \epsilon + i0^+) \right) \end{aligned} \quad (5.65)$$

$$= - \int \frac{d\epsilon}{\pi} \frac{\partial f(\epsilon)}{\partial \epsilon} \text{Im} \text{Tr} \left(M(\mathbf{k}) \ln \hat{G}(\mathbf{k}, \epsilon + i0^+) \right). \quad (5.66)$$

We emphasize that this result holds only for conserved quantities.

5.10.2 The thermodynamic potential

A simple way to determine the thermodynamic potential is by means of the Hellmann-Feynman theorem, according to which, if the Hamiltonian depends on some parameter λ , i.e. $\mathcal{H} = \mathcal{H}(\lambda)$, then the derivative of the thermodynamic potential $\Omega(\lambda)$ with respect to λ is

$$\frac{\partial \Omega(\lambda)}{\partial \lambda} = \langle \frac{\partial \mathcal{H}(\lambda)}{\partial \lambda} \rangle_\lambda, \quad (5.67)$$

where $\langle \dots \rangle_\lambda$ means quantum and thermal average with the Hamiltonian at finite λ . Let us consider for simplicity the case of interacting electrons, the cases of bosons or electrons plus bosons being a straightforward generalization. The Hamiltonian is the free electron Hamiltonian

$$\mathcal{H}_0 = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma},$$

plus the electron-electron interaction

$$\mathcal{H}_{int} = \frac{1}{2V} \sum_{\mathbf{k}\mathbf{p}\mathbf{q}} \sum_{\alpha\beta} U(\mathbf{q}) c_{\mathbf{k}+\mathbf{q}\alpha}^\dagger c_{\mathbf{p}\beta}^\dagger c_{\mathbf{p}+\mathbf{q}\beta} c_{\mathbf{k}\alpha}.$$

Let us consider now a λ -dependent Hamiltonian

$$\mathcal{H}(\lambda) = \mathcal{H}_0 + \lambda \mathcal{H}_{int},$$

⁸The exponential factor in (5.64) guarantees that the contour integral is well behaved at $\mathcal{R}e z \rightarrow -\infty$, while when $\mathcal{R}e z \rightarrow +\infty$ is the Fermi distribution function which does the job.

then, through the Hellmann-Feynman theorem, it holds that

$$\begin{aligned}\frac{\partial \Omega(\lambda)}{\partial \lambda} &= \langle \frac{\partial \mathcal{H}_{int}}{\partial \lambda} \rangle_\lambda \\ &= \frac{1}{\lambda} \frac{1}{2V} \sum_{\mathbf{k}\mathbf{p}\mathbf{q}} \sum_{\alpha\beta} \lambda U(\mathbf{q}) \langle c_{\mathbf{k}+\mathbf{q}\alpha}^\dagger c_{\mathbf{p}\beta}^\dagger c_{\mathbf{p}+\mathbf{q}\beta} c_{\mathbf{k}\alpha} \rangle_\lambda.\end{aligned}$$

One might in principle calculate directly this average value by using the fluctuation-dissipation theorem that allows to relate the average value of a four fermion operator with the sum over frequency of the imaginary part of appropriate correlation functions, that can be accessed perturbatively. Alternatively, by means of the equation of motion of the Green's function, Eq. (5.35), we can write

$$\begin{aligned}\frac{1}{2V} \sum_{\mathbf{k}\mathbf{p}\mathbf{q}} \sum_{\alpha\beta} \lambda U(\mathbf{q}) \langle c_{\mathbf{k}+\mathbf{q}\alpha}^\dagger c_{\mathbf{p}\beta}^\dagger c_{\mathbf{p}+\mathbf{q}\beta} c_{\mathbf{k}\alpha} \rangle_\lambda &= \frac{1}{2} T \sum_n \sum_{\mathbf{k}\alpha} \left[(i\epsilon_n - \epsilon_{\mathbf{k}}) G_\alpha(\mathbf{k}, i\epsilon_n) - 1 \right] e^{i\epsilon_n 0^+} \\ &= T \sum_n \sum_{\mathbf{k}} \left(G_\alpha^{(0)}(\mathbf{k}, i\epsilon_n) \right)^{-1} \left[G_\alpha(\mathbf{k}, i\epsilon_n) - G_\alpha^{(0)}(\mathbf{k}, i\epsilon_n) \right] e^{i\epsilon_n 0^+},\end{aligned}$$

having made use of the fact that

$$\lim_{\tau \rightarrow 0} \delta(\tau) = \lim_{\tau \rightarrow 0} T \sum_n e^{i\epsilon_n \tau} = T \sum_n.$$

Therefore we finally obtain that

$$\begin{aligned}\frac{\partial \Omega(\lambda)}{\partial \lambda} &= \frac{T}{2\lambda} \sum_n \sum_{\mathbf{k}\alpha} \left(G_\alpha^{(0)}(\mathbf{k}, i\epsilon_n) \right)^{-1} \left[G_\alpha(\mathbf{k}, i\epsilon_n) - G_\alpha^{(0)}(\mathbf{k}, i\epsilon_n) \right] e^{i\epsilon_n 0^+} \\ &= \frac{T}{2\lambda} \sum_n \sum_{\mathbf{k}\alpha} \Sigma_\alpha(\mathbf{k}, i\epsilon_n) G_\alpha(\mathbf{k}, i\epsilon_n) e^{i\epsilon_n 0^+},\end{aligned}\tag{5.68}$$

where the interacting Green's function and self-energy are calculated at finite λ , and we used the Dyson equation. Since for $\lambda = 0$, the thermodynamic potential is that one of free electrons, Ω_0 , that is known, we can evaluate the interacting potential $\Omega = \Omega(\lambda = 1)$ by

$$\Omega = \Omega_0 + \int_0^1 d\lambda \frac{T}{\lambda} \sum_n \sum_{\mathbf{k}} \left(G^{(0)}(\mathbf{k}, i\epsilon_n) \right)^{-1} \left[G(\mathbf{k}, i\epsilon_n) - G^{(0)}(\mathbf{k}, i\epsilon_n) \right] e^{i\epsilon_n 0^+}.$$

Now, let us define a functional $\tilde{X}[\Sigma]$ through

$$\tilde{X}[\Sigma] = -T \sum_n \sum_{\mathbf{k}\sigma} \left[\ln \left(1 - G_\sigma^{(0)}(\mathbf{k}, i\epsilon_n) \Sigma_\sigma(\mathbf{k}, i\epsilon_n) \right) + \Sigma_\sigma(\mathbf{k}, i\epsilon_n) G_\sigma(\mathbf{k}, i\epsilon_n) \right] e^{i\epsilon_n 0^+} + X[G[\Sigma]],\tag{5.69}$$

where X is the Luttinger-Ward function, see Fig. 5.33, assuming now that G is functional of Σ (we have explicitly indicated the spin label, even though each term is spin-independent). By means of (5.62) we find that

$$\begin{aligned}\frac{\delta \tilde{X}}{\delta \Sigma_\sigma} &= \frac{G_\sigma^{(0)}}{1 - G_\sigma^{(0)} \Sigma} - G - \Sigma \frac{\delta G}{\delta \Sigma_\sigma} + \frac{\delta X}{\delta \Sigma_\sigma} \\ &= \frac{G_\sigma^{(0)}}{1 - G_\sigma^{(0)} \Sigma} - G - \Sigma \frac{\delta G}{\delta \Sigma_\sigma} + \frac{\delta X}{\delta G_\sigma} \frac{\delta G_\sigma}{\delta \Sigma_\sigma} \\ &= \frac{G_\sigma^{(0)}}{1 - G_\sigma^{(0)} \Sigma} - G - \Sigma \frac{\delta G}{\delta \Sigma_\sigma} + \Sigma \frac{\delta G_\sigma}{\delta \Sigma_\sigma} \\ &= \frac{1}{\left(G_\sigma^{(0)}\right)^{-1} - \Sigma} - G.\end{aligned}$$

The last expression is nothing but the Dyson equation. This means that \tilde{X} is stationary

$$\frac{\delta \tilde{X}}{\delta \Sigma_\sigma} = 0,$$

provided G satisfies the Dyson equation. Now, once again, we multiply the interaction by a parameter λ and assume we have calculated all quantities at finite λ , so that the self-energy becomes function of λ , i.e. $\Sigma(\lambda)$. We note that

$$\frac{\partial \tilde{X}}{\partial \lambda} = \frac{\delta \tilde{X}}{\delta \Sigma} \frac{\partial \Sigma}{\partial \lambda} + \left(\frac{\partial X}{\partial \lambda} \right)_\Sigma = \left(\frac{\partial X}{\partial \lambda} \right)_\Sigma,$$

where we have assumed that Σ is the stationary point, and the last term implies that the derivative is at fixed Σ , namely one does not need to derive anymore $\Sigma(\lambda)$ with respect to λ . The only other place in which λ appears in X is in the interaction lines that are now $\lambda U(\mathbf{q})$. Since for the n -th order diagram $X^{(n)}$ there are n interaction lines, the derivative is

$$\left(\frac{\partial X^{(n)}}{\partial \lambda} \right)_\Sigma = \frac{n}{\lambda} X^{(n)}(\lambda).$$

Therefore the perturbation expansion of the derivative of X is just the same as of X itself without the $1/n$ pre-factor of the n -th order term but with a $1/\lambda$ pre-factor. Hence, it is easy to realize, see Fig. 5.33, that

$$\frac{\partial \tilde{X}}{\partial \lambda} = \left(\frac{\partial X}{\partial \lambda} \right)_\Sigma = \frac{1}{2\lambda} T \sum_n \sum_{\mathbf{k}\sigma} \Sigma_\sigma(\mathbf{k}, i\epsilon_n) G_\sigma(\mathbf{k}, i\epsilon_n). \quad (5.70)$$

Comparing with (5.68) we find that

$$\frac{\partial \Omega(\lambda)}{\partial \lambda} = \frac{\partial \tilde{X}}{\partial \lambda}. \quad (5.71)$$

Since, for $\lambda = 0$, $\tilde{X}(0) = 0$, we immediately find that, at $\lambda = 1$,

$$\begin{aligned} \Omega &= \Omega_0 + \tilde{X}[\Sigma] \\ &= \Omega_0 - T \sum_n \sum_{\mathbf{k}\sigma} \left[\ln \left(1 - G_\sigma^{(0)}(\mathbf{k}, i\epsilon_n) \Sigma_\sigma(\mathbf{k}, i\epsilon_n) \right) + \Sigma_\sigma(\mathbf{k}, i\epsilon_n) G_\sigma(\mathbf{k}, i\epsilon_n) \right] e^{i\epsilon_n 0^+} + X[G] \\ &= T \sum_n \sum_{\mathbf{k}\sigma} \left[\ln G_\sigma(\mathbf{k}, i\epsilon_n) - \Sigma_\sigma(\mathbf{k}, i\epsilon_n) G_\sigma(\mathbf{k}, i\epsilon_n) \right] e^{i\epsilon_n 0^+} + X[G], \end{aligned} \quad (5.72)$$

where we use the expression

$$\Omega_0 = T \sum_n \sum_{\mathbf{k}\sigma} \ln G_\sigma^{(0)}(\mathbf{k}, i\epsilon_n) e^{i\epsilon_n 0^+}.$$

5.10.3 The Luttinger theorem

As usually let us assume that the Hamiltonian as well as the ground state are spin-rotationally invariant, which also implies that the Green's function is spin-independent. In this case the total number of electrons per unit volume at zero temperature is

$$\begin{aligned} \frac{N}{V} &= \frac{1}{V} \sum_{\mathbf{k}} \sum_{\sigma} n_{\mathbf{k}\sigma} = -\frac{2}{V} \sum_{\mathbf{k}} \int \frac{d\epsilon}{\pi} f(\epsilon) \frac{\partial}{\partial \epsilon} \text{Arg} \ln G^{-1}(\mathbf{k}, \epsilon + i0^+) \\ &= -\frac{2}{V} \sum_{\mathbf{k}} \int_{-\infty}^0 \frac{d\epsilon}{\pi} \frac{\partial}{\partial \epsilon} \text{Arg} \ln G^{-1}(\mathbf{k}, \epsilon + i0^+) \\ &= -\frac{2}{\pi V} \sum_{\mathbf{k}} \left(\text{Arg} \ln G^{-1}(\mathbf{k}, 0 + i0^+) - \text{Arg} \ln G^{-1}(\mathbf{k}, -\infty + i0^+) \right) \\ &= -\frac{2}{\pi V} \sum_{\mathbf{k}} (\phi(\mathbf{k}, 0) - \phi(\mathbf{k}, -\infty)), \end{aligned} \quad (5.73)$$

where

$$\phi(\mathbf{k}, \epsilon) = \tan^{-1} \left(\frac{\mathcal{I}m G(\mathbf{k}, \epsilon + i0^+)}{\mathcal{R}e G(\mathbf{k}, \epsilon + i0^+)} \right) = \tan^{-1} \left(\frac{-\mathcal{I}m G^{-1}(\mathbf{k}, \epsilon + i0^+)}{\mathcal{R}e G^{-1}(\mathbf{k}, \epsilon + i0^+)} \right), \quad (5.74)$$

is the phase of the Green's function approaching the real axis from above. From Eq. (5.14) it derives that

$$\mathcal{I}m G(\mathbf{k}, \epsilon + i0^+) = -\mathcal{I}m G(\mathbf{k}, \epsilon - i0^+) = |G(\mathbf{k}, \epsilon)| \sin \phi(\epsilon) = -\pi A(\mathbf{k}, \epsilon) \leq 0,$$

which implies that ϕ is defined within $[-\pi, 0]$. For infinite frequency a constant interaction can not be effective, hence

$$\lim_{|\epsilon| \rightarrow \infty} G(\mathbf{k}, \epsilon + i0^+) = \lim_{|\epsilon| \rightarrow \infty} G^{(0)}(\mathbf{k}, \epsilon + i0^+) \rightarrow \frac{1}{\epsilon + i0^+},$$

which implies that

$$\phi(\mathbf{k}, -\infty) = \tan^{-1} \frac{0^-}{-\infty} = -\pi.$$

We will show later that, in the most common situations, $\mathcal{I}m G^{-1}(\mathbf{k}, \epsilon + i0^+ \rightarrow 0 + i0^+) \rightarrow 0^+$ so that $G^{-1}(\mathbf{k}, 0)$ is purely real hence

$$\phi(\mathbf{k}, 0) = \tan^{-1} \frac{0^-}{G^{-1}(\mathbf{k}, 0)}$$

is equal to π if $G^{-1}(\mathbf{k}, 0) < 0$ and 0 otherwise. Using these results to evaluate (5.73) we finally obtain

$$\frac{N}{V} = \frac{2}{V} \sum_{\mathbf{k}} \theta(G^{-1}(\mathbf{k}, 0)). \quad (5.75)$$

This expression, also known as *Luttinger's theorem*, states that the number of electrons is equal to the volume in the Brillouin zone which includes all momenta such that the Green's function at zero real-frequency is positive.

Remarks

Let us discuss in what cases the above result applies.

The simplest example is when the single-particle local spectral function $A(\epsilon)$ has a gap or a pseudo-gap, i.e. vanishes as a power-law, at the chemical potential, namely at $\epsilon = 0$. Since

$$A(\epsilon) = \frac{1}{V} \sum_{\mathbf{k}} A(\mathbf{k}, \epsilon),$$

and both $A(\epsilon)$ and $A(\mathbf{k}, \epsilon)$ are by definition real and positive, this implies that for any \mathbf{k} $A(\mathbf{k}, \epsilon \rightarrow 0) \rightarrow 0$, hence also $\mathcal{I}m G(\mathbf{k}, \epsilon + i0^+ \rightarrow 0 + i0^+) = 0$. Then, through (5.74), we find that

$$\phi(\mathbf{k}, 0) = \tan^{-1} \frac{0^-}{\mathcal{R}e G(\mathbf{k}, 0)}.$$

Since the sign of the real part of G is the same as that of G^{-1} , the Luttinger sum rule (5.75) is recovered. This would be for instance the case of a superconductor.

On the contrary, in the case of a metal we do expect a finite spectral function at the chemical potential $A(0) \neq 0$, so the above demonstration does not work. We notice that

$$\begin{aligned}\mathcal{R}e G^{-1}(\mathbf{k}, \epsilon + i0^+) &= \epsilon - \epsilon_{\mathbf{k}} - \mathcal{R}e \Sigma(\mathbf{k}, \epsilon + i0^+), \\ \mathcal{I}m G^{-1}(\mathbf{k}, \epsilon + i0^+) &= 0^+ - \mathcal{I}m \Sigma(\mathbf{k}, \epsilon + i0^+),\end{aligned}$$

so that the question reduces to know how it behaves the imaginary part of the self-energy upon approaching the real axis. We have already shown, see Eq. (5.27), that within perturbation theory

$$\lim_{\epsilon \rightarrow 0} \mathcal{I}m \Sigma(\mathbf{k}, \epsilon + i0^+) = 0^-,$$

which justifies the Luttinger sum rule also in this case.

Chapter 6

Landau-Fermi liquid theory: a microscopic justification

The Landau-Fermi liquid theory, that we have introduced at the beginning as a phenomenological description of the low energy excitations of an interacting electron gas, can be justified microscopically using the Feynmann diagram technique that we have just discussed.

6.1 Preliminaries

We are going to discuss the Landau-Fermi liquid theory in a model of N degenerate species of fermions, $a = 1, \dots, N$. At the moment we shall consider only short-range interactions; later we will extend the analysis to the Coulomb case. The non-interacting Green's function is defined by

$$G_a^{(0)}(\mathbf{k}, i\epsilon_n) = G^{(0)}(\mathbf{k}, i\epsilon_n) = \frac{1}{i\epsilon_n - \epsilon_{\mathbf{k}}^0},$$

and the interacting one by

$$G_a(\mathbf{k}, i\epsilon_n) = G(\mathbf{k}, i\epsilon_n) = \frac{1}{i\epsilon_n - \epsilon_{\mathbf{k}}^0 - \Sigma(\mathbf{k}, i\epsilon_n)},$$

and both are a -independent. All energies are measured with respect to the chemical potential.

We know that, provided perturbation theory is valid, the self-energy analytically continued on the real axis, $\Sigma(\mathbf{k}, \epsilon)$, has an imaginary part that vanishes at least like ϵ^2 for $\epsilon \rightarrow 0$. This implies that, for very small ϵ ,

$$G(\mathbf{k}, \epsilon) \simeq \frac{1}{\epsilon - \epsilon_{\mathbf{k}}^0 - \Re e \Sigma(\mathbf{k}, \epsilon)},$$

which we are going to assume has a simple pole on the real axis at $\epsilon = \epsilon_{\mathbf{k}}$ such that

$$\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}}^0 - \Re e \Sigma(\mathbf{k}, \epsilon_{\mathbf{k}}) = 0,$$

with residue

$$Z_{\mathbf{k}} = \left| 1 - \frac{\partial \Re e \Sigma(\mathbf{k}, \epsilon)}{\partial \epsilon} \Big|_{\epsilon=\epsilon_{\mathbf{k}}} \right|^{-1}.$$

This pole represents a particle-like coherent excitation, that has to be identified as the *quasiparticle*. The residue, which is smaller than one as the derivative of the self-energy is negative, is the weight of a quasi-particle excitation into a real particle one. By consistency, $\epsilon_{\mathbf{k}}$ must be very small, so that the imaginary part of the self-energy at $\epsilon = \epsilon_{\mathbf{k}}$ is indeed negligible with respect to $\epsilon_{\mathbf{k}}$ itself. Within this assumption, for complex frequency z very close to the origin,

$$G(\mathbf{k}, z) \simeq \frac{Z_{\mathbf{k}}}{z - \epsilon_{\mathbf{k}}} + G_{inc}(\mathbf{k}, z), \quad (6.1)$$

where $G_{inc}(\mathbf{k}, z)$ is an incoherent component that has no singularity for small $|z|$. Within this assumption, the surface identified by $\epsilon_{\mathbf{k}} = 0$ corresponds by the Luttinger theorem to the Fermi surface.

Let us now consider the Bethe-Salpeter equation (5.47), which can be written formally as

$$\Gamma = \Gamma^0 + \Gamma^0 \odot R \odot \Gamma, \quad (6.2)$$

where \odot means the sums over internal indices, including the sum over momenta and Matsubara frequencies, and

$$R(\mathbf{k}, i\epsilon_n; \mathbf{q}, i\omega_l) = G(\mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l) G(\mathbf{k}, i\epsilon_n). \quad (6.3)$$

We note that, for free electrons and for small \mathbf{q} and ω_l

$$\begin{aligned} T \sum_n G^{(0)}(\mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l) G^{(0)}(\mathbf{k}, i\epsilon_n) F(i\epsilon_n) &= T \sum_n \frac{1}{i\epsilon_n + i\omega_l - \epsilon_{\mathbf{k}+\mathbf{q}}^0} \frac{1}{i\epsilon_n - \epsilon_{\mathbf{k}}^0} F(i\epsilon_n) \\ &= \oint \frac{dz}{2\pi i} f(z) \frac{1}{z + i\omega_l - \epsilon_{\mathbf{k}+\mathbf{q}}^0} \frac{1}{z - \epsilon_{\mathbf{k}}^0} F(z) \\ &\simeq \frac{f(\epsilon_{\mathbf{k}}^0) - f(\epsilon_{\mathbf{k}+\mathbf{q}}^0)}{i\omega_l - \epsilon_{\mathbf{k}+\mathbf{q}}^0 + \epsilon_{\mathbf{k}}^0} F(\epsilon_{\mathbf{k}}^0) + \oint \frac{dz}{2\pi i} f(z) \left(\frac{1}{z - \epsilon_{\mathbf{k}}^0} \right)^2 \left(F(z) \right)_{sing} \\ &\simeq -\frac{\partial f(\epsilon_{\mathbf{k}}^0)}{\partial \epsilon_{\mathbf{k}}^0} \frac{\epsilon_{\mathbf{k}+\mathbf{q}}^0 - \epsilon_{\mathbf{k}}^0}{i\omega_l - \epsilon_{\mathbf{k}+\mathbf{q}}^0 + \epsilon_{\mathbf{k}}^0} F(\epsilon_{\mathbf{k}}^0) + \oint \frac{dz}{2\pi i} f(z) \left(\frac{1}{z - \epsilon_{\mathbf{k}}^0} \right)^2 \left(F(z) \right)_{sing} \\ &\simeq \delta(\epsilon_{\mathbf{k}}^0) \frac{\epsilon_{\mathbf{k}+\mathbf{q}}^0 + \epsilon_{\mathbf{k}}^0}{i\omega_l - \epsilon_{\mathbf{k}+\mathbf{q}}^0 + \epsilon_{\mathbf{k}}^0} F(0) + \oint \frac{dz}{2\pi i} f(z) \left(\frac{1}{z - \epsilon_{\mathbf{k}}^0} \right)^2 \left(F(z) \right)_{sing}, \end{aligned}$$

where $\left(F(z)\right)_{sing}$ means that one has to catch in the contour integral only the singularities of F . In the above equation, the term

$$\delta(\epsilon_k^0) \frac{\mathbf{v}_k^0 \cdot \mathbf{q}}{i\omega_l - \mathbf{v}_k^0 \cdot \mathbf{q}}$$

has a singular behavior for small \mathbf{q} and ω_l . If $q = 0$ and ω_l finite, it vanishes, while if $\omega_l = 0$ at finite q , it is $-\delta(\epsilon_k^0)$. In other words, the function

$$R^{(0)}(\mathbf{k}, i\epsilon_n; \mathbf{q}, i\omega_l) = G^{(0)}(\mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l) G^{(0)}(\mathbf{k}, i\epsilon_n)$$

regarded as a distribution in $i\epsilon_n$, has a singular part at small \mathbf{q} and ω_l given by

$$-\frac{\partial f(\epsilon_k^0)}{\partial \epsilon_k^0} \delta(i\epsilon_n) \frac{\mathbf{v}_k^0 \cdot \mathbf{q}}{i\omega_l - \mathbf{v}_k^0 \cdot \mathbf{q}}.$$

The formal meaning of $\delta(i\epsilon_n)$ for discrete Matsubara frequencies is

$$\delta(i\epsilon_n) = \frac{1}{T} \delta_{n0}.$$

Seemingly, the product of two interacting Green's functions of the form (6.1), regarded as a distribution, can be represented at small q and ω_l as

$$\begin{aligned} R(\mathbf{k}, i\epsilon_n; \mathbf{q}, i\omega_l) &= G(\mathbf{k} + \mathbf{q}, i\epsilon_n + i\omega_l) G(\mathbf{k}, i\epsilon_n) \\ &\simeq -\frac{\partial f(\epsilon_k)}{\partial \epsilon_k} \delta(i\epsilon_n) Z_k^2 \frac{\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}}{i\omega_l - \epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}}} + R_{inc}(\mathbf{k}, i\epsilon_n; \mathbf{q}, i\omega_l) \\ &\equiv \Delta(\mathbf{k}, i\epsilon_n; \mathbf{q}, i\omega_l) + R_{inc}(\mathbf{k}, i\epsilon_n; \mathbf{q}, i\omega_l), \end{aligned} \quad (6.4)$$

where $R_{inc}(\mathbf{k}, i\epsilon_n; \mathbf{q}, i\omega_l)$ is non-singular for $q \rightarrow 0$ and $\omega_l \rightarrow 0$, and

$$\Delta(\mathbf{k}, i\epsilon_n; \mathbf{q}, i\omega_l) = -\frac{\partial f(\epsilon_k)}{\partial \epsilon_k} \delta(i\epsilon_n) Z_k^2 \frac{\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}}{i\omega_l - \epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}}}. \quad (6.5)$$

We note that, if we send first $q \rightarrow 0$ and then $\omega_l \rightarrow 0$, so-called ω -limit, then

$$\lim_{\omega_l \rightarrow 0} \lim_{q \rightarrow 0} R = R^\omega = R_{inc}, \quad (6.6)$$

while, in the opposite case, so called q -limit,

$$\lim_{q \rightarrow 0} \lim_{\omega_l \rightarrow 0} R = R^q = \frac{\partial f(\epsilon_k)}{\partial \epsilon_k} \delta(i\epsilon_n) Z_k^2 + R_{inc} = \Delta^q + R^\omega. \quad (6.7)$$

Going back to the Bethe-Salpeter equation (6.2), we note that the irreducible vertex Γ^0 is by definition non-singular at small q and ω_l , in other words its ω -limit coincides with the q -limit. Therefore, in both limits,

$$\Gamma^q = \Gamma^0 + \Gamma^0 \odot R^q \odot \Gamma^q, \quad (6.8)$$

$$\Gamma^\omega = \Gamma^0 + \Gamma^0 \odot R^\omega \odot \Gamma^\omega, \quad (6.9)$$

with the same Γ^0 . Solving for Γ^0 we find that

$$\Gamma = \Gamma^q + \Gamma^q \odot (R - R^q) \odot \Gamma \equiv \Gamma^q + \Gamma^q \odot \tilde{\Delta} \odot \Gamma, \quad (6.10)$$

where

$$\begin{aligned} \tilde{\Delta}(\mathbf{k}, i\epsilon_n; \mathbf{q}, i\omega_l) &= \Delta(\mathbf{k}, i\epsilon_n; \mathbf{q}, i\omega_l) - \frac{\partial f(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}} \delta(i\epsilon_n) Z_{\mathbf{k}}^2 \\ &= -\frac{\partial f(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}} \delta(i\epsilon_n) Z_{\mathbf{k}}^2 \frac{i\omega_l}{i\omega_l - \epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}}}, \end{aligned} \quad (6.11)$$

or, alternatively,

$$\Gamma = \Gamma^\omega + \Gamma^\omega \odot (R - R^\omega) \odot \Gamma = \Gamma^\omega + \Gamma^\omega \odot \Delta \odot \Gamma. \quad (6.12)$$

In this way we have been able to absorb the unknown R_{inc} and Γ^0 into two scattering vertices, Γ^q and Γ^ω .

6.1.1 Vertex and Ward identities

The fermionic operators $c_{\mathbf{k}a}$, labelled by generic quantum numbers $a = 1, N$, have, as we assumed, interacting Green's functions diagonal in these numbers and independent of them. Let us now add a perturbation of the form

$$\delta\mathcal{H} = h(-\mathbf{q}) \cdot \sum_{\mathbf{k}} \sum_{ab} m_{ab}(\mathbf{k}, \mathbf{q}) c_{\mathbf{k}a}^\dagger c_{\mathbf{k}+q b} \equiv h \cdot \mathcal{M},$$

in the limit of $q \rightarrow 0$. In this limit it is convenient for what follows to rotate the basis $c_{\mathbf{k}a}$ into the one $c_{\mathbf{k}\alpha}$ that diagonalizes the matrix $\hat{m}(\mathbf{k})$ with elements $m_{ab}(\mathbf{k})$, i.e. $m_{ab}(\mathbf{k}) \rightarrow m_\alpha(\mathbf{k}) \delta_{ab}$. However, even though we are going to use this diagonal basis to derive explicitly several identities, we will always provide for each of these identities also a matrix representation, which is obviously independent of the basis set.

In the diagonal basis the non interacting Green's function is also diagonal,

$$\left(G_\alpha^{(0)}(\mathbf{k}, i\epsilon_n) \right)^{-1} = i\epsilon_n - \epsilon_{\mathbf{k}} - h m_\alpha(\mathbf{k}),$$

while the interacting one might not be so

$$(G_\alpha(\mathbf{k}, i\epsilon_n))_{\alpha\beta}^{-1} = i\epsilon_n - \epsilon_{\mathbf{k}} - h m_\alpha(\mathbf{k}) \delta_{\alpha\beta} - \Sigma_{\alpha\beta}(\mathbf{k}, i\epsilon_n). \quad (6.13)$$

If the operator \mathcal{M} refers to a conserved quantity of the fully interacting Hamiltonian, then the interacting self-energy is diagonal, hence also the Green's function.

In the presence of the external field, the average value of the operator \mathcal{M} , namely

$$\langle \mathcal{M} \rangle = \sum_\alpha m_\alpha(\mathbf{k}) n_{\mathbf{k}\alpha} = \frac{1}{V} \sum_{\mathbf{k}} T \sum_n \sum_\alpha m_\alpha(\mathbf{k}) G_{\alpha\alpha}(\mathbf{k}, i\epsilon_n),$$

becomes h dependent, which allows to define the thermodynamic susceptibility

$$\kappa = \frac{\partial \langle \mathcal{M} \rangle}{\partial h} |_{h=0} = \frac{1}{V} \sum_{\mathbf{k}} T \sum_n \sum_\alpha m_\alpha(\mathbf{k}) \frac{\partial G_{\alpha\alpha}(\mathbf{k}, i\epsilon_n)}{\partial h} |_{h=0}. \quad (6.14)$$

We note that, considering $G_{\alpha\beta}$ as elements of a matrix \hat{G} , as well as m_α of a diagonal matrix \hat{m} , and so on, the following relation holds:

$$\frac{\partial \hat{G}(\mathbf{k}, i\epsilon_n)}{\partial h} = \hat{G}(\mathbf{k}, i\epsilon_n) \left(\hat{m}(\mathbf{k}) + \frac{\partial \hat{\Sigma}(\mathbf{k}, i\epsilon_n)}{\partial h} \right) \hat{G}(\mathbf{k}, i\epsilon_n). \quad (6.15)$$

This equation is actually independent of the basis set, namely it holds also in the original representation where $\hat{m}(\mathbf{k})$ has elements $m_{ab}(\mathbf{k})$. On the other hand, through Eq. (5.58) we know that

$$\frac{\partial \Sigma_{\alpha\beta}(\mathbf{k}, i\epsilon_n)}{\partial h} = T \sum_m \sum_\gamma \frac{1}{V} \sum_{\mathbf{p}} \Gamma_{\alpha\gamma;\delta\beta}(\mathbf{k} i\epsilon_n, \mathbf{p} i\epsilon_m; \mathbf{p} i\epsilon_m, \mathbf{k} i\epsilon_n) G_{\delta\nu}(\mathbf{p}, i\epsilon_m) m_\nu(\mathbf{p}) G_{\nu\gamma}(\mathbf{p}, i\epsilon_m),$$

where the product of the two Green's functions must be interpreted as

$$\lim_{q \rightarrow 0} G_{\delta\nu}(\mathbf{p} + \mathbf{q}, i\epsilon_m) G_{\nu\gamma}(\mathbf{p}, i\epsilon_m),$$

namely as the q -limit. In the limit $h \rightarrow 0$, that we will consider hereafter, all Green's functions become diagonal and independent of the index α , i.e. $G_{\alpha\beta} = \delta_{\alpha\beta} G$, hence

$$\begin{aligned} m_\alpha(\mathbf{k}) \delta_{\alpha\beta} + \frac{\partial \Sigma_{\alpha\beta}(\mathbf{k}, i\epsilon_n)}{\partial h} |_{h=0} &= m_\alpha(\mathbf{k}) \delta_{\alpha\beta} \\ &+ T \sum_m \sum_\gamma \frac{1}{V} \sum_{\mathbf{p}} \Gamma_{\alpha\gamma;\beta\gamma}(\mathbf{k} i\epsilon_n, \mathbf{p} i\epsilon_m; \mathbf{p} i\epsilon_m, \mathbf{k} i\epsilon_n) R^q(\mathbf{p} i\epsilon_m) m_\gamma(\mathbf{p}), \end{aligned} \quad (6.16)$$

where we recall that

$$R^q(\mathbf{p} i\epsilon_m) = \lim_{q \rightarrow 0} G(\mathbf{p} + \mathbf{q}, i\epsilon_m) G(\mathbf{p}, i\epsilon_m).$$

We can also introduce the triangular vertex $\Lambda_{\alpha\beta}(\mathbf{k} + \mathbf{q} i\epsilon_n + i\omega_l, \mathbf{k} i\epsilon_n; \mathbf{q} i\omega_l)$ corresponding to the perturbation, with non-interacting value at small q

$$\Lambda_{\alpha\beta}^{(0)}(\mathbf{k} + \mathbf{q} i\epsilon_n + i\omega_l, \mathbf{k} i\epsilon_n; \mathbf{q} i\omega_l) = m_\alpha(\mathbf{k}) \delta_{\alpha\beta}.$$

As we know Λ satisfies the Bethe-salpeter equation

$$\Lambda = \Lambda^{(0)} + \Gamma \odot R \odot \Lambda^{(0)}.$$

Similarly to the above discussion of the interaction vertices, we can define the q and ω limits of the triangular vertex

$$\begin{aligned}\Lambda^q &= \Lambda^{(0)} + \Gamma^q \odot R^q \odot \Lambda^{(0)}, \\ \Lambda^\omega &= \Lambda^{(0)} + \Gamma^\omega \odot R^\omega \odot \Lambda^{(0)}.\end{aligned}$$

Solving for $\Lambda^{(0)}$ one finds that the vertex is related to its q or ω limits by

$$\Lambda = \Lambda^\omega + \Gamma^\omega \odot \Delta \odot \Lambda = \Lambda^\omega + \Gamma \odot \Delta \odot \Lambda^\omega, \quad (6.17)$$

$$\Lambda = \Lambda^q + \Gamma^q \odot \tilde{\Delta} \odot \Lambda = \Lambda^q + \Gamma \odot \tilde{\Delta} \odot \Lambda^q, \quad (6.18)$$

where Δ and $\tilde{\Delta}$ have been defined in Eqs. (6.5) and (6.11), respectively.

Through Eq. (6.16) and by the definition of the triangular vertex, we obtain the following identity:

$$\boxed{m_\alpha(\mathbf{k}) \delta_{\alpha\beta} + \frac{\partial \Sigma_{\alpha\beta}(\mathbf{k}, i\epsilon_n)}{\partial h} = \Lambda_{\alpha\beta}^q(\mathbf{k}, i\epsilon_n)}, \quad (6.19)$$

or, in a representation independent of the basis choosen,

$$\boxed{\hat{m}(\mathbf{k}) + \frac{\partial \hat{\Sigma}(\mathbf{k}, i\epsilon_n)}{\partial h} = \hat{\Lambda}^q(\mathbf{k}, i\epsilon_n)}. \quad (6.20)$$

Let us assume now that the operator \mathcal{M} is a conserved quantity, which implies that, even if $h \neq 0$, the Green's functions remain diagonal in α . In this case the Ward identity (5.56) holds, which reads in this case and for $\mathbf{q} = \mathbf{0}$

$$\begin{aligned}m_\alpha(\mathbf{k}) \frac{\Sigma_\alpha(\mathbf{k}, i\epsilon_n + i\omega_l) - \Sigma_\alpha(\mathbf{k}, i\epsilon_n)}{i\omega_l} &= -\frac{1}{V} \sum_{\mathbf{p}} T \sum_m \sum_\beta \\ \Gamma_{\alpha\beta; \beta\alpha}(\mathbf{k} i\epsilon_n, \mathbf{p} i\epsilon_m + i\omega_l; \mathbf{p} i\epsilon_m, \mathbf{k} i\epsilon_n + i\omega_l) G_\beta(\mathbf{p}, i\epsilon_m) G_\beta(\mathbf{p}, i\epsilon_m + i\omega_l) m_\beta(\mathbf{p}).\end{aligned}$$

In the limit of $\omega_l \rightarrow \omega_0 \ll 1$ we can write

$$m_\alpha(\mathbf{k}) \frac{\partial \Sigma_\alpha(\mathbf{k}, i\epsilon_n)}{\partial i\epsilon_n} = -\frac{1}{V} \sum_{\mathbf{p}} T \sum_m \sum_\beta \Gamma_{\alpha\beta; \beta\alpha}(\mathbf{k} i\epsilon_n, \mathbf{p} i\epsilon_m + i\omega_0; \mathbf{p} i\epsilon_m, \mathbf{k} i\epsilon_n + i\omega_0)$$

$$\begin{aligned} & G_\beta(\mathbf{p}, i\epsilon_m) G_\beta(\mathbf{p}, i\epsilon_m + i\omega_0) m_\beta(\mathbf{p}) \\ = & -\Lambda_{\alpha\alpha}^\omega(\mathbf{k}, i\epsilon_n) + m_\alpha(\mathbf{k}). \end{aligned} \quad (6.21)$$

In other words, another identity holds, namely:

$$m_\alpha(\mathbf{k}) - m_\alpha(\mathbf{k}) \frac{\partial \Sigma_\alpha(\mathbf{k}, i\epsilon_n)}{\partial i\epsilon_n} = \Lambda_\alpha^\omega(\mathbf{k}, i\epsilon_n), \quad (6.22)$$

or, in matrix form,

$$\hat{m}(\mathbf{k}) - \hat{m}(\mathbf{k}) \frac{\partial \hat{\Sigma}(\mathbf{k}, i\epsilon_n)}{\partial i\epsilon_n} = \hat{\Lambda}^\omega(\mathbf{k}, i\epsilon_n). \quad (6.23)$$

In the limit of vanishing \hbar and for small ϵ_n , this identity becomes

$$\hat{\Lambda}^{(0)}(\mathbf{k}) Z_{\mathbf{k}}^{-1} = \hat{\Lambda}^\omega(\mathbf{k}, i\epsilon_n). \quad (6.24)$$

We emphasize that this result holds only for a conserved operator.

6.2 Correlation functions

Two single particle operators

$$\mathcal{A}(\mathbf{q}) = \sum_{\mathbf{k}} \sum_{ab} c_{\mathbf{k}a}^\dagger \Lambda_{Aab}^{(0)}(\mathbf{k}, \mathbf{q}) c_{\mathbf{k}+q b}, \quad \mathcal{B}(\mathbf{q}) = \sum_{\mathbf{k}} \sum_{ab} c_{\mathbf{k}a}^\dagger \Lambda_{Bab}^{(0)}(\mathbf{k}, \mathbf{q}) c_{\mathbf{k}+q b},$$

can be associated to a correlation function $\chi_{AB}(\mathbf{q}, i\omega_l)$ that is defined by

$$\chi_{AB} = \text{Tr}\left(\Lambda_A^{(0)} R \Lambda_B^{(0)}\right) + \text{Tr}\left(\Lambda_A^{(0)} R \Gamma R \Lambda_B^{(0)}\right) = \text{Tr}\left(\Lambda_A^{(0)} R \Lambda_B\right), \quad (6.25)$$

where all quantities are calculated at zero external fields.¹ Once more we can define q and ω limits by (we drop for simplicity the subscripts A and B , keeping in mind that the triangular vertex on the left refers to A , and that one on the right to B):

$$\chi^\omega = \text{Tr}\left(\Lambda^{(0)} R^\omega \Lambda^\omega\right),$$

¹The actual meaning of the trace over the internal indices α 's is

$$\begin{aligned} \text{Tr}\left(\Lambda_A^{(0)} R \Lambda_B\right) &= \sum \Lambda_{A\alpha\beta}^{(0)} G_{\beta\gamma} \Lambda_{B\gamma\delta} G_{\delta\alpha} \\ &= \sum \Lambda_{A\alpha\beta}^{(0)} G^2 \Lambda_{B\beta\alpha} \end{aligned}$$

since at zero field the Green's functions are diagonal and independent of α .

$$\chi^q = \text{Tr}(\Lambda^{(0)} R^q \Lambda^q).$$

Through Eqs. (6.17) and (6.18), we can rewrite (6.25) in the following way:

$$\begin{aligned}\chi &= \text{Tr}[\Lambda^{(0)} R (\Lambda^\omega + \Gamma \Delta \Lambda^\omega)] = \text{Tr}(\Lambda^{(0)} R \Lambda^\omega) + \text{Tr}(\Lambda^{(0)} R \Gamma \Delta \Lambda^\omega) \\ &= \text{Tr}(\Lambda^{(0)} R^\omega \Lambda^\omega) + \text{Tr}[\Lambda^{(0)} (R - R^\omega) \Lambda^\omega] + \text{Tr}(\Lambda^{(0)} R \Gamma \Delta \Lambda^\omega) \\ &= \chi^\omega + \text{Tr}(\Lambda^{(0)} \Delta \Lambda^\omega) + \text{Tr}(\Lambda^{(0)} R \Gamma \Delta \Lambda^\omega) \\ &= \chi^\omega + \text{Tr}(\Lambda \Delta \Lambda^\omega) \\ &= \chi^\omega + \text{Tr}[(\Lambda^\omega + \Lambda^\omega \Delta \Gamma) \Delta \Lambda^\omega] \\ &= \chi^\omega + \text{Tr}(\Lambda^\omega \Delta \Lambda^\omega) + \text{Tr}(\Lambda^\omega \Delta \Gamma \Delta \Lambda^\omega).\end{aligned}\tag{6.26}$$

Similarly, it also holds that

$$\chi = \chi^q + \text{Tr}(\Lambda^q \tilde{\Delta} \Lambda^q) + \text{Tr}(\Lambda^q \tilde{\Delta} \Gamma \tilde{\Delta} \Lambda^q).\tag{6.27}$$

We note that both $\Delta(\mathbf{k}, i\epsilon_n; \mathbf{q}, i\omega_l)$ and $\tilde{\Delta}(\mathbf{k}, i\epsilon_n; \mathbf{q}, i\omega_l)$ contain a delta function in frequency, $\delta(\epsilon_n)$ and a derivative of the Fermi function with respect to its argument. This implies first that all sums over the internal Matsubara frequencies drop out, all frequencies being fixed to the lowest one $\epsilon_0 = \pi T$, and that all momenta are very close to the Fermi surface. We define, for small q and ω_l

$$\lambda_k^\omega = Z_k \Lambda^\omega(\mathbf{k}, 0; \mathbf{q} = \mathbf{0}, i\omega_l \rightarrow 0),\tag{6.28}$$

$$\lambda_k^q = Z_k \Lambda^q(\mathbf{k}, 0; \mathbf{q} \rightarrow \mathbf{0}, i\omega_l = 0),\tag{6.29}$$

$$A_{\mathbf{kp}}(\mathbf{q}, i\omega_l) = Z_k Z_p \Gamma(\mathbf{k} + \mathbf{q} 0 + i\omega_l, \mathbf{p} 0; \mathbf{p} + \mathbf{q} 0 + i\omega_l, \mathbf{k} 0),,\tag{6.30}$$

$$f_{\mathbf{kp}} = Z_k Z_p \Gamma^\omega(\mathbf{k} 0, \mathbf{p} 0; \mathbf{p} 0, \mathbf{k} 0),\tag{6.31}$$

as well as

$$\delta_{\mathbf{k}}(\mathbf{q}, i\omega_l) = -\frac{\partial f(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}} \frac{\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}}{i\omega_l - \epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}}},\tag{6.32}$$

$$\tilde{\delta}_{\mathbf{k}}(\mathbf{q}, i\omega_l) = -\frac{\partial f(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}} \frac{i\omega_l}{i\omega_l - \epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}}}.\tag{6.33}$$

With these definitions,

$$A = f + f \odot \delta \odot A,\tag{6.34}$$

and Eqs. (6.26) and (6.27) can be written as

$$\chi(\mathbf{q}, i\omega_l) = \chi^\omega + \text{Tr}(\lambda^\omega \delta \lambda^\omega) + \text{Tr}(\lambda^\omega \delta A \delta \lambda^\omega)$$

$$= \chi^q + \text{Tr}(\lambda^q \tilde{\delta} \lambda^q) + \text{Tr}(\lambda^q \tilde{\delta} A \tilde{\delta} \lambda^q), \quad (6.35)$$

where the trace does not include anymore the sum over Matsubara frequencies. The explicit expressions read

$$\begin{aligned} \chi(\mathbf{q}, i\omega_l) &= \chi^\omega - \frac{1}{V} \sum_{\mathbf{k}} \sum_{\alpha\beta} \lambda_{\mathbf{k}\alpha\beta}^\omega \lambda_{\mathbf{k}\beta\alpha}^\omega \frac{\partial f(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}} \frac{\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}}{i\omega_l - \epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}}} \\ &\quad + \frac{1}{V^2} \sum_{\mathbf{k}\mathbf{p}} \sum_{\alpha\beta\gamma\delta} \frac{\partial f(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}} \frac{\partial f(\epsilon_{\mathbf{p}})}{\partial \epsilon_{\mathbf{p}}} \lambda_{\mathbf{k}\alpha\beta}^\omega A_{\mathbf{k}\beta, \mathbf{p}\gamma; \mathbf{p}\delta, \mathbf{k}\alpha}(\mathbf{q}, i\omega_l) \lambda_{\mathbf{p}\delta\gamma}^\omega \\ &\quad \frac{\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}}{i\omega_l - \epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}}} \frac{\epsilon_{\mathbf{p}+\mathbf{q}} - \epsilon_{\mathbf{p}}}{i\omega_l - \epsilon_{\mathbf{p}+\mathbf{q}} + \epsilon_{\mathbf{p}}} \end{aligned} \quad (6.36)$$

$$\begin{aligned} &= \chi^q - \frac{1}{V} \sum_{\mathbf{k}} \sum_{\alpha\beta} \lambda_{\mathbf{k}\alpha\beta}^q \lambda_{\mathbf{k}\beta\alpha}^q \frac{\partial f(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}} \frac{i\omega_l}{i\omega_l - \epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}}} \\ &\quad + \frac{1}{V^2} \sum_{\mathbf{k}\mathbf{p}} \sum_{\alpha\beta\gamma\delta} \frac{\partial f(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}} \frac{\partial f(\epsilon_{\mathbf{p}})}{\partial \epsilon_{\mathbf{p}}} \lambda_{\mathbf{k}\alpha\beta}^q A_{\mathbf{k}\beta, \mathbf{p}\gamma; \mathbf{p}\delta, \mathbf{k}\beta}(\mathbf{q}, i\omega_l) \lambda_{\mathbf{p}\delta\gamma}^q \\ &\quad \frac{i\omega_l}{i\omega_l - \epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}}} \frac{i\omega_l}{i\omega_l - \epsilon_{\mathbf{p}+\mathbf{q}} + \epsilon_{\mathbf{p}}}. \end{aligned} \quad (6.37)$$

We just note that, through Eqs. (6.20), (6.13) and (6.15), we can relate χ^q

$$\begin{aligned} \chi^q &= \frac{1}{V} \sum_{\mathbf{k}} T \sum_n \text{Tr} \left[\Lambda_A^{(0)}(\mathbf{k}, \mathbf{0}) G(\mathbf{k}, i\epsilon_n) \left(\Lambda_B^{(0)}(\mathbf{k}, \mathbf{0}) + \frac{\partial \Sigma(\mathbf{k}, i\epsilon_n)}{\partial h_B} \Big|_{h=0} \right) G(\mathbf{k}, i\epsilon_n) \right] \\ &= \frac{1}{V} \sum_{\mathbf{k}} T \sum_n \text{Tr} \left[\Lambda_A^{(0)}(\mathbf{k}, \mathbf{0}) \frac{\partial G(\mathbf{k}, i\epsilon_n)}{\partial h_B} \Big|_{h=0} \right] = \kappa_{AB}, \end{aligned}$$

to the thermodynamic susceptibility, κ_{AB} , of the operator \mathcal{A} to an external field h_B that couples to \mathcal{B} . So far we have been able to express any correlation function in a form similar to that of free particles (quasi-particles), with R replaced by the “free-particle” quantities δ and $\tilde{\delta}$, all interaction effects being absorbed into the unknown three- and four-leg vertices. However, when both \mathcal{A} and \mathcal{B} refer to conserved quantities, a lot of simplifications arise.

6.2.1 Conserved quantities

Suppose that \mathcal{A} is conserved (the same result would hold if \mathcal{B} , or both were conserved). Then

$$\chi_{AB}^\omega = \text{Tr} \left(\Lambda_A^\omega R^\omega \Lambda_B^{(0)} \right).$$

Through Eq. (6.23), we find that²

$$\begin{aligned}\chi_{AB}^\omega &= \frac{1}{V} \sum_{\mathbf{k}} T \sum_n \text{Tr} \left[\Lambda_A^{(0)}(\mathbf{k}, \mathbf{q} = \mathbf{0}) \left(1 - \frac{\partial \Sigma(\mathbf{k}, i\epsilon_n)}{\partial i\epsilon_n} \right) G(\mathbf{k}, i\epsilon_n + i\omega_l) G(\mathbf{k}, i\epsilon_n) \Lambda_B^{(0)}(\mathbf{k}, \mathbf{q} = \mathbf{0}) \right] \\ &= \frac{1}{V} \sum_{\mathbf{k}} \text{Tr} \left[\Lambda_A^{(0)}(\mathbf{k}, \mathbf{q} = \mathbf{0}) \Lambda_B^{(0)}(\mathbf{k}, \mathbf{q} = \mathbf{0}) \right] T \sum_n \frac{\partial G(\mathbf{k}, i\epsilon_n)}{\partial i\epsilon_n} = 0,\end{aligned}\quad (6.38)$$

namely χ_{AB}^ω vanishes. Therefore, by means of Eq. (6.24), we finally obtain, when both \mathcal{A} and \mathcal{B} are conserved, and for small q and ω_l ,

$$\begin{aligned}\chi_{AB}(\mathbf{q}, i\omega_l) &= -\frac{1}{V} \sum_{\mathbf{k}} \sum_{ab} \Lambda_{Aab}^{(0)}(\mathbf{k}, \mathbf{0}) \Lambda_{Bba}^{(0)}(\mathbf{k}, \mathbf{0}) \frac{\partial f(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}} \frac{\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}}{i\omega_l - \epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}}} \\ &\quad + \frac{1}{V^2} \sum_{\mathbf{kp}} \sum_{\alpha\beta} \Lambda_{Aab}^{(0)}(\mathbf{k}, \mathbf{0}) A_{\mathbf{k}b, \mathbf{p}c; \mathbf{p}d, \mathbf{k}a} \Lambda_{Bdc}^{(0)}(\mathbf{k}, \mathbf{0}) \\ &\quad \frac{\partial f(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}} \frac{\partial f(\epsilon_{\mathbf{p}})}{\partial \epsilon_{\mathbf{p}}} \frac{\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}}{i\omega_l - \epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}}} \frac{\epsilon_{\mathbf{p}+\mathbf{q}} - \epsilon_{\mathbf{p}}}{i\omega_l - \epsilon_{\mathbf{p}+\mathbf{q}} + \epsilon_{\mathbf{p}}}.\end{aligned}\quad (6.39)$$

We immediately recognize that the above expression coincides with that one obtained within the Landau-Fermi-liquid theory, in the general case of quantum numbers $a = 1, \dots, N$. Therefore, when considering conserved quantities, all interaction effects can be absorbed into the quasiparticle energy $\epsilon_{\mathbf{k}}$ and into the scattering vertices A .

6.3 Coulomb interaction

So far we have only taken into account short-range electron-electron interaction. What does it change when the interaction is instead long-ranged?

Let us assume therefore that the electrons interact mutually by a long-range Coulomb repulsion

$$\mathcal{H}_{int} = \frac{1}{V} \sum_{\mathbf{kpq}} \sum_{ab} U(\mathbf{q}) c_{\mathbf{k}+\mathbf{qa}}^\dagger c_{\mathbf{pb}}^\dagger c_{\mathbf{p}+qb}^\dagger c_{\mathbf{ka}}^\dagger,$$

with

$$U(\mathbf{q}) = \frac{4\pi e^2}{q^2}.$$

Furthermore we shall assume that there is a background positive charge that compensate exactly the electron one. This implies that the self-energy, see Fig. 5.19, does not include the Fock term, which otherwise would give an infinite contribution since $U(\mathbf{q} \rightarrow \mathbf{0}) \rightarrow \infty$. The problem with

²Recall that at zero field the Green's functions $G_{ab} = \delta_{ab} G$.

a long-range interaction is that, besides the singular behavior for small q and ω_l due to R , additional singularities arise at $q \rightarrow 0$ by the interaction. In order to disentangle both sources of singularities, it is convenient to adopt the same approach as in section 5.6.

Therefore, in the perturbative expansion of the four-leg vertex $\Gamma(\mathbf{k} + \mathbf{q}, \mathbf{p}; \mathbf{p} + \mathbf{q}, \mathbf{k})$, we identify a subset of proper diagrams that do not include any interaction line with momentum \mathbf{q} . This subset defines the proper vertex $\tilde{\Gamma}$, which by definition does not include any singularity for $\mathbf{q} \rightarrow \mathbf{0}$ arising from the singular behavior of $U(\mathbf{q})$. The proper vertex allows to define a proper density-density correlation function³

$$\tilde{\chi} = \text{Tr}(R) + \text{Tr}\left(R\tilde{\Gamma}R\right),$$

as well as a proper three-leg vertex

$$\tilde{\Lambda} = \Lambda^{(0)} + \tilde{\Gamma} \odot R \odot \Lambda^{(0)}.$$

By exploiting the analytical properties of R , we can follow precisely what we did before, this time for proper vertices. Notice that, since the self-energy does not include the Fock-term, all vertex and Ward identities still hold in terms of proper vertices. In particular, the expression (6.39) remains valid for the proper correlation function with

$$A_{\mathbf{kp}} = Z_{\mathbf{k}} Z_{\mathbf{p}} \tilde{\Gamma}^{\omega}(\mathbf{k}, \mathbf{p}; \mathbf{p}, \mathbf{k}).$$

Once we have been able to express proper correlation functions in terms of few parameters, the improper ones can be derived straightforwardly just like in section 5.6. The results obviously coincide with the Landau-Silin theory.

³Note that in the charge-density channel the non-interacting vertex $\Lambda_{ab}^{(0)} = \delta_{ab}$.